

Annual
Report
2012

CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich



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Welcome from the Director



Thomas Schulthess, Director of CSCS.

Welcome to this CSCS review of 2012 – a decisive year for our centre.

The data centre construction project in Lugano was completed on schedule and within budget, and CSCS moved into the new building. Much has been written about this project in previous reports and all that remained for 2012 was to complete the facility tests and relocate the entire CSCS' operations to the new buildings. The relocation, however, was not a regular one with movers loading and unloading boxes containing all manner of items. Instead, it involved relocating complex IT equipment that has to function in concert with the building infrastructure and, moreover, various basic services (e.g. network and data repositories) had to be available at all times during the move. Furthermore, the various systems had to be installed and returned to operation in a totally new data centre that is literally an order of magnitude more capable, but also more complex. This scale-up will have a profound impact on CSCS, affecting our organisation in many more ways than simply pure supercomputer performance. Most importantly, however, it will provide the Swiss scientific computing community with incredible opportunities to grow in both quality and quantity.

The Swiss University Conference also decided to fund the Platform for Advanced Scientific Computing (PASC) as one of its structuring projects during the fiscal period 2013–2016. The platform organises and implements domain science networks that have ambitious scientific agendas and will drive the development of future supercomputing systems built at CSCS.

This will have profound impact on the development processes at CSCS and positions the centre as an attractive partner for the computer industry in the co-design of future simulation systems.

Finally, the respective Executive Boards of ETH Zurich and the EPFL approved and signed a collaboration framework that will allow CSCS to host the supercomputing systems of the Blue Brain Project. Since the venture is Switzerland's contribution to the Human Brain Project (HBP), a European flagship project on future and emerging technologies in ICT, CSCS is now well positioned as the host site for the development systems for the HBP. Clearly, this will serve to strengthen CSCS' co-design strategy further and provide a European platform for the development of future simulation systems.

I would like to thank all CSCS staff, ETH Zurich, the University of Lugano (USI), as well as all the people and organisations that have supported us in recent years, especially in 2012. We are excited about the future and what the coming years will bring, particularly 2013, which will see us construct a new generation of supercomputers, begin hosting the next generation systems for the Blue Brain project and launch the first co-design projects within PASC.

Prof. Thomas Schulthess
Director of CSCS

A handwritten signature in blue ink, reading "TSchulthess".

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2013 will be remembered as the year the European Union and the USA officially recognised brain research as big science. On 28 January, European Commissioner Nellie Kroes announced a billion euros of funding for the Swiss-led Human Brain Project (HBP) – a massive ten-year project that aims not just to model and simulate the complete human brain but, equally importantly, use the knowledge gained to fight brain disease and develop new brain-inspired computing technologies. Just one week later, the American press reported what could be an even larger, US-led project to develop a complete description of the activity of the brain – a Brain Activity Map. In this project, too – which in many ways complements the Human Brain Project – the proposers are not only interested in neuroscience but also its applications in medicine and computing. Neither of the two projects would be conceivable without modern high-performance computing. Both have the potential to give back at least as much as they take.



Henry Markram is the Human Brain Project coordinator and leads the HBP Brain Simulation Division. (Image: EPFL)

In years to come, brain research will be an important driver for the development of high-performance computing technologies, often anticipating the needs of other applications. Particularly significant are the needs of brain modelling and simulation, which will drive high-performance computing research and development in at least three distinct areas.

The first will be memory architectures. The human brain contains some 80 billion neurons, each with its own distinctive morphology, electrical behaviour, molecular make-up and connectivity. Representing this complexity in models and simulating their dynamics will require hundreds of petabytes of random access memory.

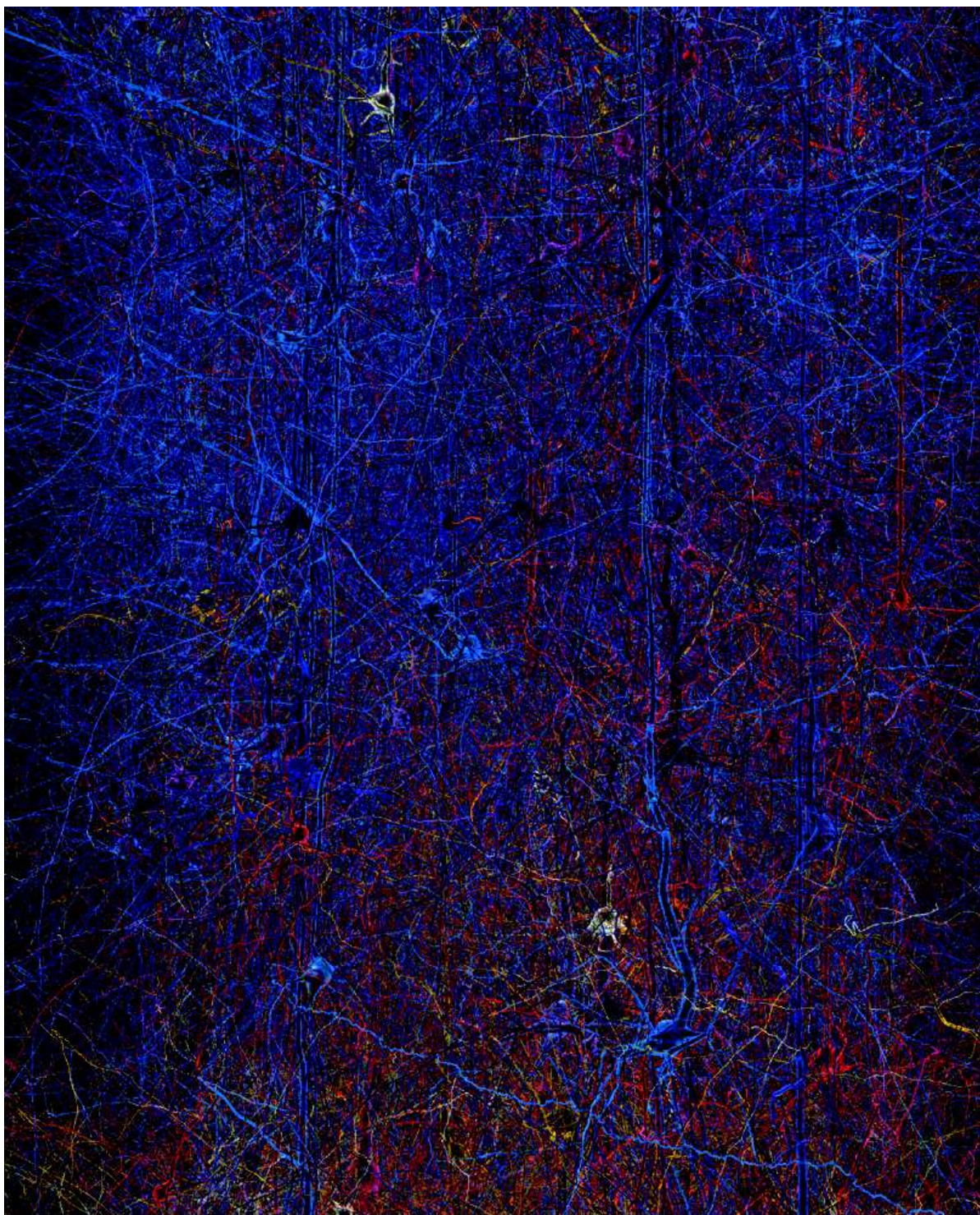
Brain simulation will thus give a major impulse to the development of new memory architectures that complement expensive DRAM – the mainstay of current systems – with less expensive memory technologies.

A second extremely important area of research will be interactive supercomputing – a completely new way of operating supercomputers that allows scientists to visualise and “steer” simulations as they run – a precondition for *in silico* experimentation.

Yet another issue is strong scaling: how to deal with computational problems – often found in brain simulation – which require very fast computation but are not susceptible to classical parallelisation. Large-scale brain simulation is likely to require custom hardware and architectures – a shift away from the current emphasis on generic machines. Neuromorphic technologies derived from knowledge of actual brain circuitry could provide some of the solutions.

The Human Brain Project will address these challenges, both through research and the design and deployment of a high-performance computing platform that will supply the project with the computing capabilities it requires, evolving step-wise towards exascale capabilities. The platform will be designed, procured and operated by four leading actors in European high-performance computing – Jülich Supercomputing Centre, which will operate the project’s “production machine”; the Barcelona Supercomputing Centre, which will provide computing capabilities for the project’s effort in Molecular Dynamics; CINECA, in Italy, which will provide capabilities for compute-intensive data analysis; and CSCS, the project’s main development centre.

CSCS’s involvement in the Human Brain Project began with the centre’s participation in the HBP Preparatory Study – the successful EU-funded Coordinating Action that paved the way for today’s flagship project. Since then, CSCS has worked closely with the EPFL to design the supercomputing infrastructure for the Blue Brain Project, which will be responsible for the HBP’s Brain Simulation Platform. In 2012 the ETH Board identified the Blue Brain Project as a national research infrastructure, commissioning CSCS and EPFL to design and deploy the necessary supercomputing capabilities. The work is making rapid progress: today, just one year after receiving the mandate from the board, CSCS has successfully procured the machine that the EPFL will use to develop the next generation of simulation tools. We look forward to many years of fruitful collaboration.



1000 "pyramidal cells" (a type of neurone) during a network simulation. Blue cells are silent and red cells are firing. (Image: EPFL/ Blue Brain Project)



KEY INFORMATION

Founded in 1991, the Swiss National Supercomputing Centre, CSCS, develops and promotes technical and scientific services for the Swiss research community in the field of high-performance computing. CSCS enables world-class scientific research by pioneering, operating and supporting leading-edge supercomputing technologies.

Largest Production Machine

Monte Rosa, Cray XE6, 402 TFlops
47 872 Cores, 46 TB Memory

Computing Time for Science

2012: 270 922 127 CPU hrs
2011: 177 201 383 CPU hrs

User Community

2012: 83 Projects, 842 Users
2011: 80 Projects, 704 Users

Employees

2012: 54
2011: 51

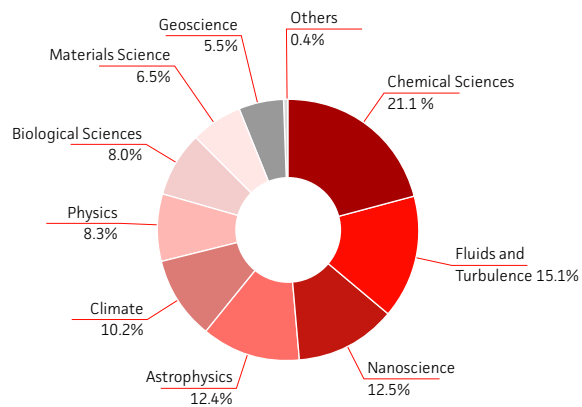
Investments

2012: 17.3 Mio CHF
2011: 15.8 Mio CHF

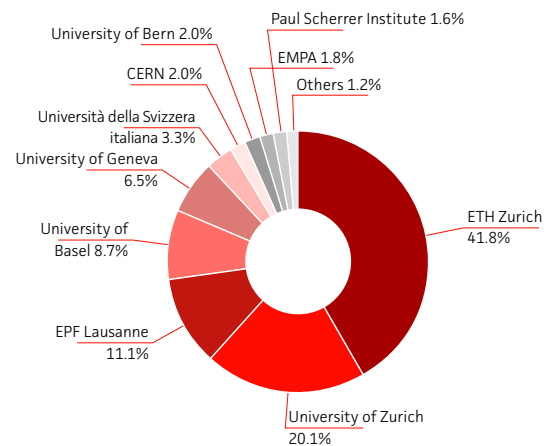
Operational Costs

2012: 11.9 Mio CHF
2011: 11.9 Mio CHF

Usage by Research Field



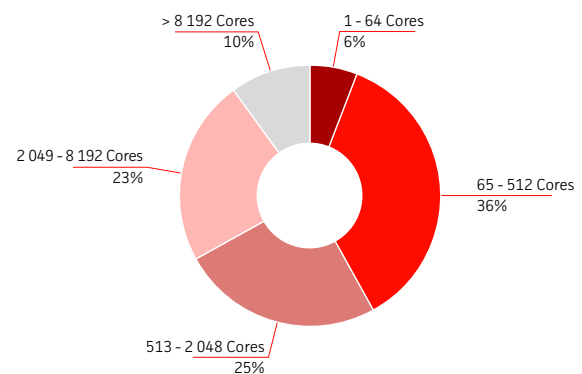
Usage by Institution



Computing Systems

Name	Supplier & Model	Installation / Upgrade	Usage / Customer	Peak Performance (TFlops)
Monte Rosa	Cray XE6	2009 / 2011	National User Lab	402.0
Tödi	Cray XK7	2010 / 2012	National User Lab, R&D	393.0
Castor	IBM iDataPlex Cluster	2011 / 2012	R&D	46.7
Monte Lema	Cray XE6	2012	MeteoSwiss	33.9
Phoenix	Sun Cluster	2007 / 2012	CHIPP (LHC Grid)	21.5
Albis	Cray XE6	2012	MeteoSwiss	16.5
Pilatus	Intel Sandy Bridge Cluster	2012	National User Lab	14.0
Eiger	Dalco Cluster	2010 / 2011	Visualisation	10.2
Piz Julier	IBM / Transtec Cluster	2010 / 2011	National User Lab	3.3
Rothorn	SGI Altix UV 1000	2011	National User Lab	2.7
Matterhorn	Cray XMT2	2011	National User Lab	–

Usage by Number of Cores per Job



January

Deployment of a data disaster recovery infrastructure

“Hope for the best, prepare for the worst”, as the saying goes. The data produced by researchers running simulations on CSCS systems is stored on “project”, a shared parallel file system based on IBM GPFS software that is accessible from all CSCS computers. Data allowances are granted for the entire duration of a project.

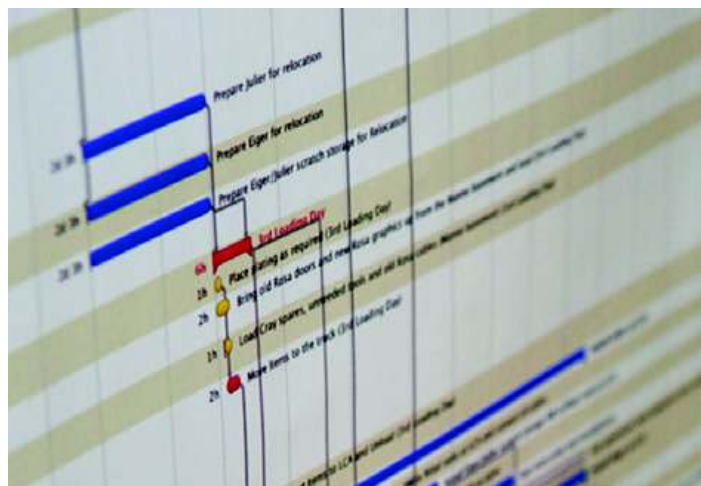
By the end of 2011, “project” already contained one petabyte of data and 20 million files, and three terabytes were moved or changed every day. At that stage, however, there was still no file system backup in place to handle such a huge amount of data. In the event of a severe accident, the results of months of simulation could well have been lost, a risk that nobody was prepared to take.

In January, a new disaster recovery infrastructure was installed that allows one to recover the file structure from metadata within just two hours and the most critical files within two days. Full data recovery should be possible within two to three weeks. The deployed solution is based on IBM software and an LTO tape storage system. It promises to scale well and thus will be ready for future data growth and storage needs.

Planning the relocation to the new building

It was early January when CSCS system engineers completed their detailed plans of how to move all computer systems and related infrastructure to the new building in Lugano-Corona. The actual move began in late March and took about four months to complete. Computers were simply shut down, switched off, packed up and moved, while certain services (e.g. file systems) were moved “online”, i.e. without interruption, through the temporary utilisation of redundant systems at the old and new locations.

Cray certainly played an important role in shifting all Cray systems, assuring a smooth transition of production services to the new building. Several tons of equipment were moved, some as complete racks and others as individual items. The amount of work invested in the move is best illustrated with the relocation of the storage infrastructure: nearly 2,000 hard drives had to be removed from their high-density enclosures and packed separately to ensure safe shipping.



System engineers planning the relocation.

February

Most efficient cluster worldwide to analyse data from CERN

Since 2010 CSCS has been operating the Phoenix cluster for the Swiss Institute of Particle Physics (CHIPP), which is used to analyse data from three of the four Large Hadron Collider (LHC) detectors: ATLAS, CMS and LHCb.

The ATLAS team periodically runs tests (“HammerCloud tests”) to compare the data analysis efficiencies of various computer systems installed all over the globe. Phoenix has outperformed all the other competitors in these tests by a remarkable 20% margin.



ATLAS installation team.
(Image: ATLAS Experiment © 2012 CERN)

March

Staff relocates to the building

In early March CSCS started its move from the old location in Manno to the new building in Lugano. The first to relocate were the employees not involved in operating supercomputers. Technical staff and supercomputers followed by the end of March.

A “housewarming party” in February preceded the actual move, providing employees and their relatives with the opportunity to visit the new building and view the future offices and computer rooms.

Maria Grazia Giuffreda (Head of User Support) describes her first impressions of the new building: “I am truly impressed by what advanced construction technology and environmentally friendly design have been able to achieve. Not only does the new building draw upon the natural lake water resource to cope with the ever-present cooling problem that large supercomputer centres face; it has become both a functional and beautiful workplace”.



General Manager Dominik Ulmer and artist of the wooden sculpture in the foyer.

“The spacious, still almost empty machine room is inspiring. Free of pillars, with no obstacles obstructing your view, it is there to remind you to open your mind, take a deep breath and leap into the future.

I literally see the new supercomputer centre as a fresh beginning for CSCS, a culmination of the intense efforts over the past few years that offers us the prospect of a challenging and rewarding adventure into future generations of supercomputing.”

John Biddiscombe (Computer Scientist) also commented on his first impressions: “My initial impressions of the structure and quality were good: huge spacious windows to let light in, efficient heating with automatic computer-controlled blinds, glass wind buffers around the structure – all the trimmings one would expect from a modern design; a machine room so cavernous that it evokes visions of the Mines of Moria (though without the trolls we hope), large enough to host Olympic events and racks of equipment – connected to the offices via an elevated space-age walkway. Strings of smoke detectors dangle from the machine room ceiling like holiday bunting, allowing the pinpoint detection of any problems should they arise; light switches fitted with LCD screens for the precise control of every watt of illumination – everything about the building smacks of the 21st century and we are left with a feeling of awe that this is our new home (and yes, we do sometimes work long into the night).”

HPC Advisory Council Switzerland Conference 2012

The HPC Advisory Council and the Swiss National Supercomputing Centre co-organised the HPC Advisory Council Switzerland Conference for the third time, which was held in the Lugano Convention Centre again this year on 13-15 March.

The conference focused on high speed networks, high performance and parallel I/O, communication libraries, (MPI, SHMEM, PGAS), GPU computing, CUDA, OpenCL, and “big data”, bringing together system managers, researchers, developers, computational scientists, students and industry affiliates for cross-training and to discuss recent HPC developments and future advancements.

More than 120 HPC specialists attended the conference, making Lugano the European HPC capital for three consecutive days.

April

Spring allocation for proposals

CSCS’ first allocation period in 2012 started on 1 April. A total of 218 million CPU hours were granted to forty new proposals and twenty-six renewals.



Participants in the Workshop on Big Data and Graph Analysis.

May

Workshop on Big Data and Graph Analysis inaugurates new conference room

The conference room in the new centre was inaugurated in May with a workshop on Big Data and Graph Analysis on the Cray uRIKA “Matterhorn”. The speakers were John Feo and Oreste Villa of Pacific Northwest National Laboratory and Jim Maltby of Cray, Inc.

The Cray uRIKA graph appliance addresses the challenge of delivering insightful analytics on graphs, not only in terms of its ability to handle the size and complexity of relationships, but also its response time and processing speed.

The aim of the workshop was to teach potential users about the functionalities offered by this machine and give them an opportunity to discuss their specific computational or data analysis problems with experts.

2012 Cray User Group: Best Paper Award

One of CSCS staff members, Dr Tim Robinson, won the Best Paper Award at the 2012 Cray User Group (CUG) meeting in Stuttgart. The paper, entitled *Software usage on Cray systems across three centres (NICS, ORNL and CSCS)*, resulted from a collaboration with Oak Ridge National Laboratory and the National Institute for Computational Sciences, Tennessee.

It describes the implementation of a software tool to determine the usage of numerical libraries, compilers and applications automatically and transparently, right down to the level of specific version numbers.

The tool allows HPC centres to monitor software usage and forecast needs – to determine which compiler suites are most used and should continue to be supported in the future, for instance. Moreover, the tool can alert support staff to situations where a user is running code that is linked to legacy or deprecated libraries or, even worse, libraries known to be buggy.

June

“Nicola goes to Berkeley”

CSCS has established an exchange program that allows employees to visit peer centres and learn about the various approaches in the high-performance computing (HPC) business.

CSCS system engineer Nicola Bianchi spent five weeks at the National Energy Research Scientific Computing Center (NERSC) in Berkeley, California.

During his sojourn, Nicola entertained his colleagues at CSCS with a fun and humorous blog on his experiences. More importantly, however, he returned with many new ideas to share with them.



Lake Merritt near NERSC: Nicola and his new colleagues used to run around the lake during the lunch breaks. (Image: Nicola Bianchi)

Upon his return, Nicola commented: "Working with such skilled and experienced people helped me to understand that there is always a different way to solve a problem or approach a project. And yes, also that even if you think you're a geek, there's always someone geekier than you!"

CSCS co-organises and hosts the PRACE Summer School on Code Optimisation for Multi-Core and Intel MIC Architectures

On 21-23 June CSCS hosted the PRACE Summer School on Code Optimisation for Multi-Core and Intel MIC Architectures. Participants came from many different countries all over Europe and the rest of the world.

On the first day, CSCS and EPCC (Edinburgh Parallel Computing Centre) staff gave lectures on modern x86 vectorisation, cache and multi-core performance tuning. On the second day, Intel technical staff conducted specific training on the Intel MIC architecture and the programming techniques required to exploit the new systems. The final day was used to demonstrate numerical libraries and MPI on MIC systems and discuss early user experiences of the Texas Advanced Computing Center (TACC) and the National Institute for Computational Sciences (NICS). Throughout the school's hands-on sessions, PRACE participants were given the world's first public access to Intel's Knights Corner MIC processors.

July

Shutdown of last supercomputer in Manno ends twenty years of history

The last CSCS supercomputer to be switched off in Manno was Piz Buin, a Cray XT4, which served MeteoSwiss for five years to compute the numerical weather forecast once every three hours, utilising simulations based on the COSMO model.

The move from Manno to Lugano began at the end of March and was formally completed only three months later with the shutdown of Piz Buin. In spite of a very ambitious schedule, the move went smoothly and all milestones were completed on time. The impact on the end users was minimised: Monte Rosa, the largest production system, was off line for just two weeks, the GPFS file system was always available and not a single run of the numerical weather forecast was lost. This was only made possible thanks to the unwavering commitment of CSCS staff and their external service providers.

A short film published on YouTube documents how CSCS system engineer Davide Tacchella, in an almost empty computer room, sends the final shutdown command to turn off Piz Buin and thus complete a twenty-year chapter in the history of supercomputing in Manno. Pushing the button was an emotional moment, but it also marked the beginning of an exciting new era of Swiss supercomputing in Lugano.

Albis and Monte Lema: two new supercomputers for MeteoSwiss

By mid-June MeteoSwiss started to use two new Cray XE6 systems, Albis and Monte Lema, which replaced Piz Buin and its backup La Dôle soon afterwards as MeteoSwiss' only computing resource to produce weather forecasts for Switzerland.



Albis & Monte Lema, the new Cray XE6 systems at CSCS.

The production system, Albis, is a single cabinet Cray XE6 with 1,728 computing cores. Monte Lema, the backup and development system, is made up of two cabinets with 4,032 computing cores.

The names Albis and Monte Lema were chosen because MeteoSwiss operates two of its three Swiss meteorological radar stations on these mountains (the third one being on La Dôle).



A system engineer working on the Cray XE6 systems.

August

Summer School on Parallel Programming and Scalable Performance Analysis

From 6-8 August CSCS hosted a three-day summer school on parallel programming geared towards graduate students who were new to high-performance computing and wished to learn the basic skills required to write, develop and maintain parallel applications in scientific computing.

The topics included the principles of parallel programming, distributed memory programming with MPI, shared memory programming with OpenMP and hybrid programming with MPI/OpenMP. On all three days, a large portion of time was dedicated to lab sessions.

Inauguration of new CSCS building by Federal Councillor Alain Berset

Read the special feature for the full story (pag. 44).

September

Over 2,000 visitors attend CSCS Open Day

Read the special feature for the full story (pag. 45).

Over 100 meteorologists convene in Lugano for the COSMO General Meeting

For a week, the city of Lugano saw meteorologists from all over Europe come together for the COSMO General Meeting. COSMO stands for Consortium for Small-Scale Modelling, which develops and maintains the numerical weather prediction application that is used by many European national weather services. The choice of Lugano as the venue was certainly thanks to MeteoSwiss, which was a founding member of COSMO, and the strong collaboration with CSCS, which operates the MeteoSwiss systems and runs the COSMO application.

As a sponsor of this event, CSCS invited meteorologists to visit its brand new computer centre in Lugano and some of CSCS staff joined the participants for a dinner on a charming boat cruise on the Lake Lugano.

User Day 2013

After several years in Lucerne, the annual CSCS User Day meeting has returned to the computer centre, now in Lugano. At the same time, the event has been extended from one to two days to allow for presentations from both the user community and CSCS. For the second year, users were invited to show posters on their research and advertise them in two-minute presentations.



Participants at the User Day 2012 in Lugano.

The speakers invited were professors Petros Koumotsakos and Nicola Spaldin from ETH Zurich, PhD student David Daverio from the University of Geneva and Dr Jim Maltby from Cray, Inc. The participants voted on the best poster and the “User Day 2012 Best Poster Award” went to Anna Possner, a PhD student in Professor Schär’s group at ETH Zurich, for her poster on cloud-resolving climate simulations.

October

CSCS offers monthly guided visits to the public

Following the enormous success of the Open Day, CSCS has decided to offer additional opportunities for the public to visit the centre. And hence, on one evening every month, CSCS will be opening its doors again. Visits start with a presentation of the centre, explaining the various services rendered and how CSCS staff contribute, and end with a guided walk through the machine and infrastructure rooms.



Participants in a guided tour of the machine and infrastructure rooms.

Autumn allocation for Proposals

CSCS’ second allocation period in 2012 started on 1 October. A total of 53 million additional CPU hours were granted to nineteen new proposals.

USI and CSCS host hpc-ch forum on how to handle huge amounts of data for HPC

The hpc-ch community meets twice a year to discuss recent HPC developments and best practices.

The community was established to support and foster the exchange of knowledge between HPC providers and users in Switzerland. It has become a tradition for one of the two annual meetings to be hosted by CSCS and the Università della Svizzera italiana (USI).

The October meeting focused on how the HPC community should deal with huge amounts of data. Many scientific fields rely on increasingly large data sets. Depending on the discipline, this data may come either from measurement (e.g. in astrophysics, genomics) or simulation (e.g. climate research).

The challenge for HPC providers is to offer a solution to handle petabytes or even exabytes of data and provide an efficient way to store and use them as needed. This task requires an approach that balances bandwidth, capital investments, operational costs, security, availability and reliability – to name but a few.

With more than forty-five participants, this meeting has been the largest in the hpc-ch community since the first one was held three years ago.

November

Tödi ranks fourth in the Green500 list

The new “Green500” list was published on 14 November at the SC12 conference in Salt Lake City, USA. The excellent ranking of CSCS’ Cray XK7 Tödi was a pleasant surprise, finishing as the fourth most energy-efficient system behind only two Intel systems (Beacon, National Institute for Computational Sciences/University of Tennessee, USA, and SANAM, King Abdulaziz City for Science and Technology in Riyadh, Saudi Arabia) and Titan, the only other Cray XK7 at Oak Ridge National Laboratory, in Tennessee, USA.



Series of scientific conferences for the general public

The Open Day 2012 was a huge success, not only in terms of the sheer number of people that came to visit CSCS, but also the interest that visitors expressed in the popular science talks given by renowned researchers.

In addition to introducing the monthly guided visits, CSCS has thus decided to organise a seminar series for the general public, too, featuring talks about the importance of supercomputers and their use in the various scientific disciplines. The speakers invited are typically scientists from Swiss research institutes and universities who use CSCS computational resources to carry out their research.

Well-known seismologist and Professor Domenico Giardini launched the seminar series. On 25 January 2013, Dr Diego Rosinelli gave a presentation on computational fluid dynamics. Professor Günther Dissertori from ETH Zurich, like the first two speakers, agreed to talk about particle physics in March and Professor Angelo Auricchio (Cardiocentro Ticino) will show how supercomputers can help to cure heart problems in June.



An audience with seismologist and Professor Domenico Giardini.

December

Course on “Getting the best out of multi-core”

“Getting the best out of multi-core” was the final training course offered by CSCS in 2012. The three-day, hands-on course took a profound look into Intel Sandy Bridge and AMD Interlagos programming and presented techniques such as code vectorisation, tuning for the cache hierarchy and multi-threading. The course also included a discussion of how these techniques apply to new architectures such as the Intel Xeon Phi (a.k.a. MIC - Many Integrated Core).

A next-generation supercomputer arrives at CSCS: the Cray XC30 “Piz Daint”

The Cray XC30 arrived at CSCS on 5 December 2012. After just a few days of assembly, it found its place in the new CSCS computer room, complementing the existing systems. It was christened “Piz Daint” after the prominent peak in the Swiss part of the Ortler Alps in Grisons.

With a total of twelve cabinets, Piz Daint is the largest Cray XC30 delivered and assembled so far. It is a new-generation Cray supercomputer based on Intel processors.



Piz Daint, the Cray XC30 at CSCS.



A detail of Monte Rosa, the 16 cabinet Cray XE6 system. (Image: ETH-Rat/ Michael Sieber, Langnau/ Zürich)

The year of the move

During the first half of 2012, CSCS relocated from its old home in Manno to the new building in Lugano. Overall, the move went quite smoothly, thanks in no small part to the extraordinary teamwork of all CSCS employees. Personnel not immediately responsible for any of the supercomputers were the first to move, followed by those overseeing the operation of a particular system along with the latter. Proceeding in stages meant that CSCS remained operational almost throughout the entire relocation. Machine downtimes proved to be fairly short, two and a half weeks for Monte Rosa being the longest, and special efforts were made to ensure that the user home file system remained up without any interruption.

The personnel relocation started in early March, followed by the first batch of computers (Tödi [Cray XK6, now Cray XK7], Matterhorn [Cray XMT], Gele [internal test system]) on 20 March and the second batch, including the flagship computer Monte Rosa [Cray XE6], Piz Julier [IBM x3850], and Eiger [Dalco visualization system]) on 26 March. Moreover, the MeteoSwiss service was provided without any interruption, as their “old” system Piz Buin was not moved at all and not shut down for good until 2 July, several weeks after the replacement system, Albis, was installed at the new location and put into operation. The decommissioning of Piz Buin closed a twenty-year chapter of supercomputing history in Manno.

Resources allocated in 2012

The move did not affect the well-rehearsed process of granting computer time, from the initial call for scientific proposals to their submission, review, panel decision and final grant allocation. A total of 71 new proposals and 26 renewals were submitted in 2012, including 46 for the allocation period starting on 1 April, and 25 for the allocation period starting on 1 October. 59 proposals were successful and twelve were rejected following a technical and scientific evaluation.

The newly approved proposals were granted a total of 177 million core hours p.a. on Monte Rosa, distributed as follows: chemical sciences (21%), computational fluid dynamics (15%), nanoscience (13%), astrophysics (12%), climate science (10%), physics and biological sciences (8% each). A total of 13% was allocated to various projects in material science and geoscience. Of the 59 proposals that passed the review process, 17 were from ETH Zurich, 11 from the Università della Svizzera Italiana, 10 from the University of Zurich and 8 from EPF Lausanne. The Paul Scherrer Institute and the University of Basel contributed three each, the University of Geneva two and the University of Bern and the EMPA one each. The remaining three proposals were from universities abroad that engage in collaborations with Swiss institutions.

Even though the number of successful projects fell from 72 the previous year to 59 in 2012, the allocation increased significantly (from 111 million to 178 million core hours granted), showing that the computational needs per project continue to rise. This observation reflects the increasing complexity of computational projects and confirms a trend that we have already observed in previous years.

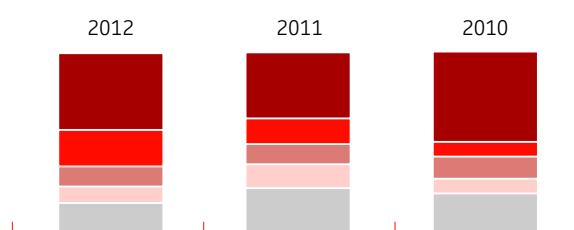
10 Largest Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in core hrs
Christoph Schär	ETH Zurich	Climate	Regional climate modeling on european and alpine scale	16.43
Leonhard Kleiser	ETH Zurich	Fluids and Turbulence	Noise emission and vortex breakdown in round subsonic jets	13.00
Petros Koumoutsakos	ETH Zurich	Fluids and Turbulence	Optimization of shape and motion patterns of single and multiple aquatic swimmers	12.00
Petros Koumoutsakos	ETH Zurich	Fluids and Turbulence	Energy cascade in high reynolds number vortical flows	12.00
Joost VandeVondele	University of Zurich	Chemical Sciences	Applications of novel ab initio MD and Monte Carlo methods	11.00
Andreas Hauser	University of Geneva	Chemical Sciences	Photophysics and photochemistry of transition metal compounds: theoretical approaches / magnetic properties of the compounds [Co(bpy) ₃][Li _x Na _{1-x} Rh(ox) ₃]	10.25
Stefan Goedecker	University of Basel	Nanoscience	Structure prediction of clusters, solids and surfaces	10.00
Juerg Hutter	University of Zurich	Chemical Sciences	Boron nitride nanomesh for guided self-assembly of molecular arrays in solution	8.40
Laurent Villard	EPF Lausanne	Plasma Physics and Fusion Energy	ORB5-TURBULENCE	8.00
Ali Alavi	University of Cambridge	Chemical Sciences	Full CI quantum Monte Carlo study of the homegeneous electron gas	7.00

Usage Statistics

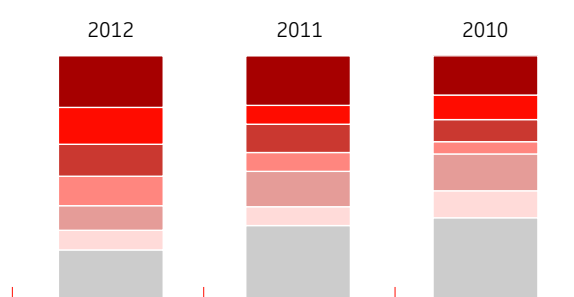
Usage by Institution (%)

Institution	2012	2011	2010
ETH Zurich	42	36	49
University of Zurich	20	14	8
EPF Lausanne	11	11	12
University of Basel	9	13	8
Others	18	26	23
Total Usage	100	100	100



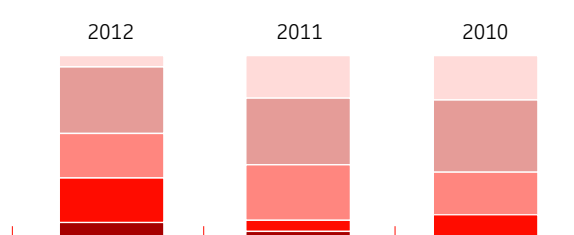
Usage by Research Field (%)

Research Field	2012	2011	2010
Chemical Sciences	21	21	16
Fluids and Turbulence	15	8	10
Nanoscience	13	12	9
Astrophysics	12	8	5
Climate	10	15	15
Biological Sciences	8	8	11
Others	21	32	34
Total Usage	100	100	100



Usage by Number of Cores per Job (%)

Cores	2012	2011	2010
1 - 256	6	23	24
257 - 1 024	36	36	39
1 025 - 4 096	25	30	23
4 097 - 16 384	23	6	12
> 16 384	10	5	2
Total Usage	100	100	100



List of Projects by Institution

EMPA

Applied nanoscience: novel catalysts and bottom-up design of graphenelike nanostructures. Computational insight within a surface science laboratory, Daniele Passerone (Nanoscience, 2.20 Mio CPU h)

EPF Lausanne

Energetic particle physics in magnetically confined configurations, Anthony W. Cooper (Plasma Physics, 2.12 Mio CPU h)

Characterization of the bacterial membrane and its interaction with antimicrobial peptides, Matteo Dal Peraro (Biological Sciences, 2.20 Mio CPU h)

First principles design and engineering of electronic and thermal transport – from nanoelectronics devices to novel thermoelectrics, Nicola Marzari (Materials Science, 2.00 Mio CPU h)

Defect levels at interfaces of high-mobility semiconductors through hybrid density functionals, Alfredo Pasquarello (Computational Condensed Matter Physics, 1.60 Mio CPU h)

Complex and reduced order structural models for blood-flow simulations, Alfio Quarteroni (Fluids and Turbulence, 1.45 Mio CPU h)

Scalable preconditioners for the Navier-Stokes equations, Alfio Quarteroni (Fluids and Turbulence, 2.65 Mio CPU h)

Simulation of plasma turbulence in the edge of tokamak devices, Paolo Ricci (Plasma Physics and Fusion Energy, 3.20 Mio CPU h)

Spin-orbit effects in Dirac fermion materials, Oleg Yazyev (Nanoscience, 1.50 Mio CPU h)

ETH Zurich

Cosmological simulations of the formation of realistic spiral galaxies, Marcella Carollo (Astrophysics, 1.50 Mio CPU h)

Low frequency wave motion as efficient energy transport in carbon nanomaterials at high heat flux, Ming Hu (Nanoscience, 2.50 Mio CPU h)

Exact diagonalization study of the fractional quantum hall effect, Sergei Isakov (Materials Science, 3.70 Mio CPU h)

Numerical simulation of particle-laden multi-phase flows, Leonhard Kleiser (Fluids and Turbulence, 3.40 Mio CPU h)

SILENS - subcritically bifurcating instability of the leading-edge boundary layer investigated by numerical simulations, Leonhard Kleiser (Fluids and Turbulence, 1.75 Mio CPU h)

Optimization of shape and motion patterns of single and multiple aquatic swimmers, Petros Koumoutsakos (Fluids and Turbulence, 12.00 Mio CPU h)

Energy cascade in high Reynolds number vortical flows, Petros Koumoutsakos (Fluids and Turbulence, 12.00 Mio CPU h)

Quantum transport simulations of nanoelectronic devices, Mathieu Luisier (Nanoscience, 5.00 Mio CPU h)

Turbulent motions inside galaxy clusters, Francesco Miniati (Astrophysics, 3.00 Mio CPU h)

Adsorption mechanisms and reactivity of H₂O and ethanol on the (110) surface of SnO₂, TiO₂ and their solid solutions, Gianluca Santarossa (Chemical Sciences, 1.00 Mio CPU h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Materials Science, 1.00 Mio CPU h)

Massively parallel multilevel Monte Carlo finite volume simulations for uncertainty quantification in nonlinear wave propagation, Christoph Schwab (Applied Mathematics, 2.20 Mio CPU h)

3-D spherical simulations of mantle convection and plate tectonics: influence of a free surface and buoyant continents, Paul Tackley (Geoscience, 1.53 Mio CPU h)

Study dynamics of ultra-cold atoms using time-dependent density-functional theory, Matthias Troyer (Materials Science, 4.00 Mio CPU h)

Image-based analyses of bone structure and function, Harry van Lenthe (Biomedical Engineering, 2.00 Mio CPU h)

Precessionally driven turbulence and dynamos in spheroidal and cylindrical enclosures, Stijn Vantieghem (Geoscience, 4.00 Mio CPU h)

Hydrocean

Simulation of ship survivability under wave impact by simulation with SPH_flow, David Guibert (Fluids and Turbulence, 0.75 Mio CPU h)

Paul Scherrer Institute

Thermodynamic equilibrium in cement from molecular simulations, Sergey Churakov (Materials Science, 0.60 Mio CPU h)

Theoretical nano-optics for photocathodes and nano-optical systems, Benedikt Oswald (Nanoscience, 1.20 Mio CPU h)

The atomistic modeling of size effects in nanocrystalline metals, Helena van Swygenhoven (Materials Science, 1.50 Mio CPU h)

Università della Svizzera italiana

Characterization of conformational dynamics and allosteric interactions in Abl kinase, Francesco Barducci (Chemical Sciences, 1.64 Mio CPU h)

Simulation of phase change materials with hybrid functionals, Sebastiano Caravati (Materials Science, 2.21 Mio CPU h)

Ab-initio molecular dynamics studies of the (H₂O)₆ water cluster, Jérôme Cuny (Chemical Sciences, 1.50 Mio CPU h)

Ab-initio molecular dynamics and metadynamics studies of the Mo₆X₁₄ (X = F, Cl, Br) molybdenum cluster in aqueous solution, Jérôme Cuny (Chemical Sciences, 1.00 Mio CPU h)

Simulation of large scale conformational fluctuations in Adenylate Kinase, Elena Formoso (Chemical Sciences, 0.90 Mio CPU h)

Investigating DNA G-quadruplex/drug interactions through enhanced sampling simulations, Vittorio Limongelli (Biological Sciences, 0.40 Mio CPU h)

Structural and conformational requisites in the folding process of the DNA quadruplex Thrombin Binding Aptamer (TBA), Michele Parrinello (Biological Sciences, 1.55 Mio CPU h)

Conformational landscape of the $\beta 2$ - $\alpha 2$ loop in prion proteins – a metadynamics study, Michele Parrinello (Biological Sciences, 1.15 Mio CPU h)

Electrophysiology of heart failure, Mark Potse (Medical/Life Science, 0.72 Mio CPU h)

Molecular simulation of nucleation and growth of molecular crystals, Gareth Tribello (Chemical Sciences, 1.10 Mio CPU h)

University of Basel

3D simulation of the aftermath of neutron star mergers and its connection to the neutrino-driven wind, Rubén Cabezón (Astrophysics, 1.50 Mio CPU h)

Structure prediction of clusters, solids and surfaces, Stefan Goedecker (Nanoscience, 10.00 Mio CPU h)

3D numerical models for magnetohydrodynamic core-collapse supernovae, Nicolas Vasset (Astrophysics, 1.51 Mio CPU h)

University of Bern

Assessing climate variability from 800 to 2100 AD and decadal predictability, Christoph Raible (Climate, 3.50 Mio CPU h)

University of Cambridge

Full CI quantum Monte Carlo study of the homogeneous electron gas, Ali Alavi (Chemical Sciences, 7.00 Mio CPU h)

University of Geneva

Photophysics and photochemistry of transition metal compounds: theoretical approaches/Magnetic properties of the compounds [Co(bpy)₃][Li_xNa_{1-x}Rh(ox)₃], Andreas Hauser (Chemical Sciences, 10.25 Mio CPU h)

Large field-theory simulations of cosmic strings, Martin Kunz (Astrophysics, 4.80 Mio CPU h)

University of Oxford

Fundamental studies on the role of nuclear quantum effects on proton/hydroxide transfer in liquid water, Michele Ceriotti (Chemical Sciences, 1.00 Mio CPU h)

University of Zurich

Simulating the effects of a preheated universe on the baryon content of galaxies, Michael Busha (Astrophysics, 5.00 Mio CPU h)

The galactic halo in mixed dark matter cosmologies, Jürgen Diemand (Astrophysics, 0.50 Mio CPU h)

Fundamental study of complex behavior of carbon materials, Rustam Khaliullin (Materials Science, 3.50 Mio CPU h)

From ERIS to UltraERISBH: co-evolution of galaxies and super-massive black holes in state-of-the-art cosmological hydro-dynamical simulations, Lucio Mayer (Astrophysics, 2.00 Mio CPU h)

Turbulence in star formation: from molecular clouds to primordial minihalos, Thomas Peters (Astrophysics, 3.00 Mio CPU h)

Simulating spiral galaxies through cosmic time, Rok Roškar (Astrophysics, 6.00 Mio CPU h)

Cosmic structure formation beyond LCDM: the warm dark matter cosmic web, Robert Smith (Astrophysics, 2.00 Mio CPU h)

The physics of galaxy clusters, Romain Teyssier (Astrophysics, 3.00 Mio CPU h)

Applications of novel ab initio MD and Monte Carlo methods, Joost VandeVondele (Chemical Sciences, 11.00 Mio CPU h)

Charge transport across a molecular switch, Laura Zoppi (Materials Science, 0.75 Mio CPU h)

Renewals

EPF Lausanne

Large-scale simulations of carbon nanotubes for NANOTERA device applications, Wanda Andreoni (Nanoscience, 4.40 Mio CPU h)

Molecular dynamics simulations of DNA minicircles, John Maddocks (Multiscale Mathematical Modelling, 1.96 Mio CPU h)

Study of land-atmosphere interaction over complex terrain by large Eddy simulation, Marc Parlange (Geoscience, 2.40 Mio CPU h)

Mixed quantum mechanical/molecular mechanical (QM/MM) studies of biological systems, Ursula Röthlisberger (Chemical Sciences, 3.82 Mio CPU h)

ORB5-TURBULENCE, Laurent Villard (Plasma Physics and Fusion Energy, 8.00 Mio CPU h)

Application of large-Eddy simulation to atmospheric boundary layer flows, Fernando Porté-Agel (Geoscience, 2.00 Mio CPU h)

ETH Zurich

Computational science and engineering in nanoelectronics, Ciappa Mauro (Nanoscience, 2.00 Mio CPU h)

Development of dynamic rupture models to study the physics of earthquakes and near-source ground motion, Luis Dalguer (Geoscience, 3.18 Mio CPU h)

Low viscosity rotating flows and magnetic field generation in Earth's core, Andrew Jackson (Geoscience, 4.80 Mio CPU h)

Role of anthropogenic versus natural forcing on decadal scales in global climate models, Ulrike Lohmann (Climate, 4.40 Mio CPU h)

Regional climate modeling on European and alpine scale, Christoph Schär (Climate, 16.43 Mio CPU h)

Land-climate interactions: modelling and analysis, Sonia Senéviratne (Climate, 0.68 Mio CPU h)

Direct numerical simulations of heat transfer and catalytic combustion in three-dimensional channels, Christos Frouzakis (Combustion, 1.80 Mio CPU h)

Direct numerical simulation of flow, heat transfer, and auto-ignition in engine-like geometries, Christos Frouzakis (Combustion, 2.00 Mio CPU h)

Noise emission and vortex breakdown in round subsonic jets, Leonhard Kleiser (Fluids and Turbulence, 13.00 Mio CPU h)

Conformational study of p38 alpha MAP kinase in free and ligand bound forms, Michele Parrinello (Biological Sciences, 1.00 Mio CPU h)

Simulating integrin junctions under tension: from the extracellular matrix to the cytoskeleton, Viola Vogel (Biological Sciences, 3.98 Mio CPU h)

Paul Scherrer Institute

Simulation of actinide materials, Matthias Krack (Materials Science, 1.30 Mio CPU h)

University of Geneva

Molecular modeling of functional anion- π complexes, Jiri Mareda (Chemical Sciences, 0.40 Mio CPU h)

University of Basel

Structure, dynamics, and function of membrane transport proteins, Simon Bernèche (Biological Sciences, 2.76 Mio CPU h)

Sensitivity of multi-dimensional supernova models with respect to nuclear input physics, Matthias Liebendörfer (Astrophysics, 1.80 Mio CPU h)

The role of dimerization in protein activation and signalling, Markus Meuwly (Chemical Sciences, 0.25 Mio CPU h)

University of Bern

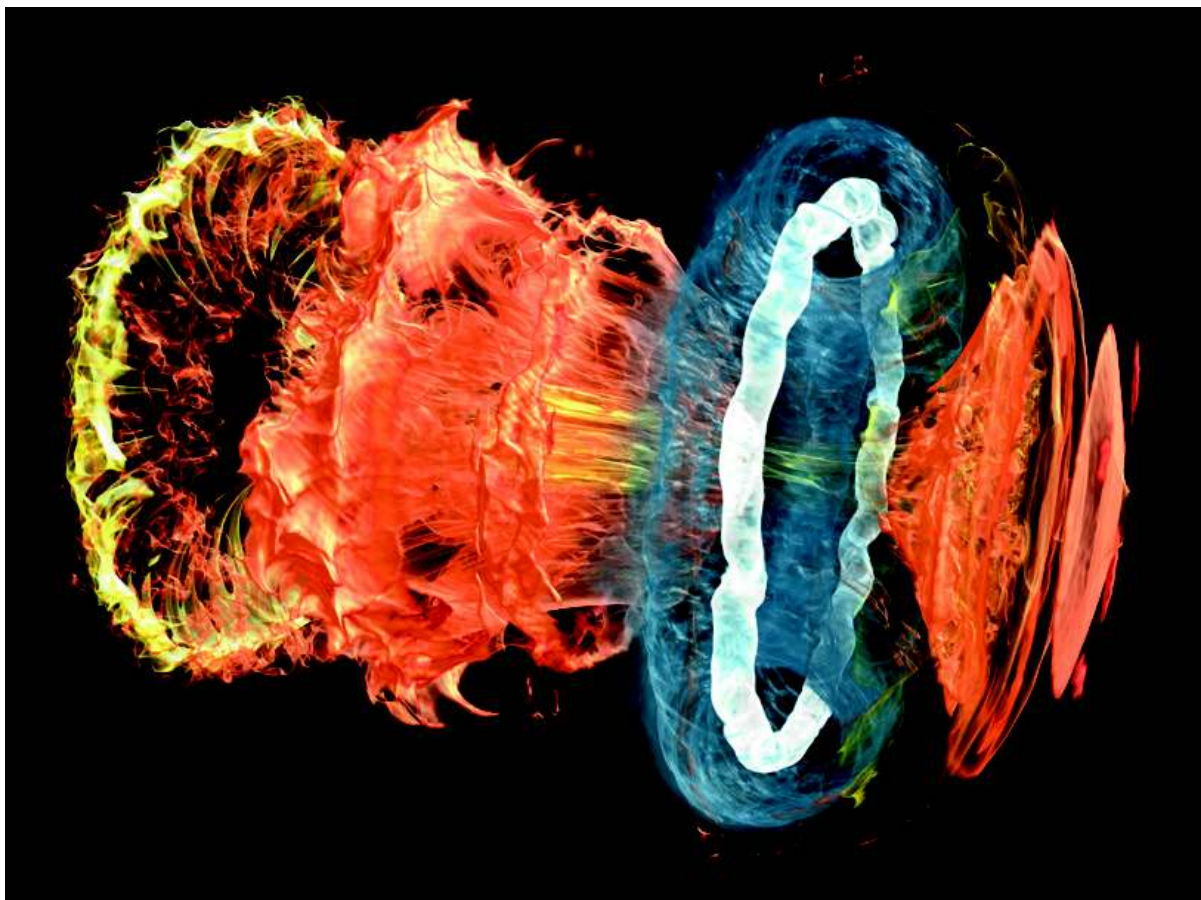
CARBOFEED (modelling carbon cycle climate feedbacks), Fortunat Joos (Climate, 0.80 Mio CPU h)

Achievements of MONALISA III, Christoph Raible (Climate, 1.16 Mio CPU h)

University of Zurich

CP2K program development, Jürg Hutter (Chemical Sciences, 1.20 Mio CPU h)

Boron nitride nanomesh for guided self-assembly of molecular arrays in solution, Jürg Hutter (Chemical Sciences, 8.40 Mio CPU h)



Volume-rendered density field of late-time shock-bubble interactions at $M=3$. Orange/ blue denote high/ low density values. (Image: Hejazialhosseini B., Rossinelli D., Conti C., Koumoutsakos P., High throughput software for direct numerical simulations of compressible two-phase flows, SC '12 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, IEEE Computer Society Press, 2012)

Searching for defects in space

Topological defects in space may have developed fractions of a second after the Big Bang. Simulations of these wormlike entities and a comparison of the simulations with cosmic background radiation measurements by the Planck satellite should confirm their existence.

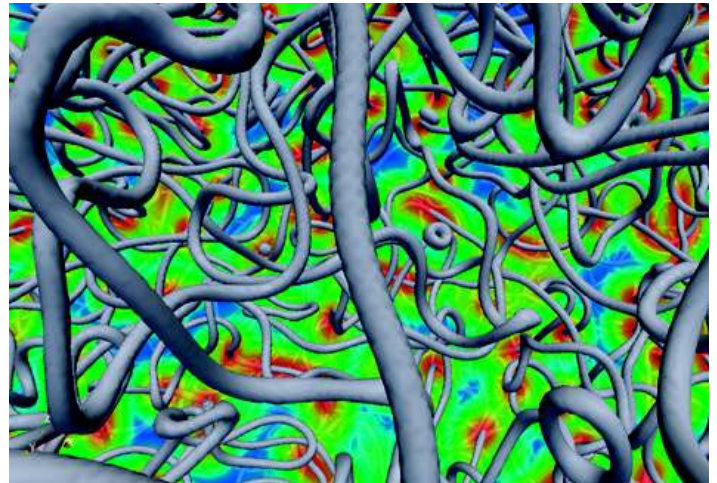
When Martin Kunz, a professor in the Cosmology Group at the University of Geneva, and his team at CSCS commandeered “Monte Rosa”, they mean business. Hardly any other computer job gets a look-in on CSCS supercomputer as it works to ninety per cent of its capacity. At least this is what the Life graph on system usage reveals. Hardly surprising when you consider that the scientists are looking to simulate a particular moment in the origin of the universe when complex mechanisms and all manner of scales played a key role: the point when topological defects, so-called “cosmic strings” to be precise, might have formed.

Smaller than a trillionth the size of a hydrogen atom

Topological defects are a common phenomenon in solid-state physics: if an area of a crystal does not undergo phase transition, in other words reorganisation in the crystal lattice, during crystallisation, a topological defect develops in the lattice. To put it simply, in cosmology topological defects are supposed to form where a phase transition occurs in the universe. This was supposedly the case a few fractions of a second after the Big Bang. The phase transition caused different basic states to develop in different areas of the cosmos. Wherever the different field conditions ultimately met, topological defects such as cosmic strings were able to form. They are supposed to be less than a trillionth the size of a hydrogen atom in diameter and quasi one-dimensional – “quasi” because, despite their defined one-dimensionality, they supposedly extend through space almost infinitely and as extremely thin “worms”. In theory, these worms weigh about twenty per cent of the Earth’s mass per kilometre in length.

Resurgence of cosmic strings

Kunz already examined topological defects in his dissertation under Geneva cosmology professor Ruth Durrer, where he endeavoured to use them to explain where the fluctuations one sees in the cosmic background radiation and out of which structures such as galaxies or galaxy clusters develop come from. However, his and other studies revealed that this does not work. “After that, topological defects were dead and buried in cosmology for a while,” says the Geneva professor.



A view through the simulated universe, gained at CSCS supercomputer “Monte Rosa”. The image shows cosmic strings (in grey) and the field density (in colour on a plane through the simulation box). Most of the strings form a tangled network, but they can also build string loops that were chopped off the long strings through intersections. (Image: David Daverio, University of Geneva, using simulation data obtained at CSCS)

It was not until cosmic inflation models became ingrained in the theories of particle physics that cosmologists began to focus on cosmic strings again. “People realised that cosmic strings are mostly produced when inflation is integrated in standard particle physics,” says Kunz. “The existence of the defects can thus be motivated far more effectively with inflation.”

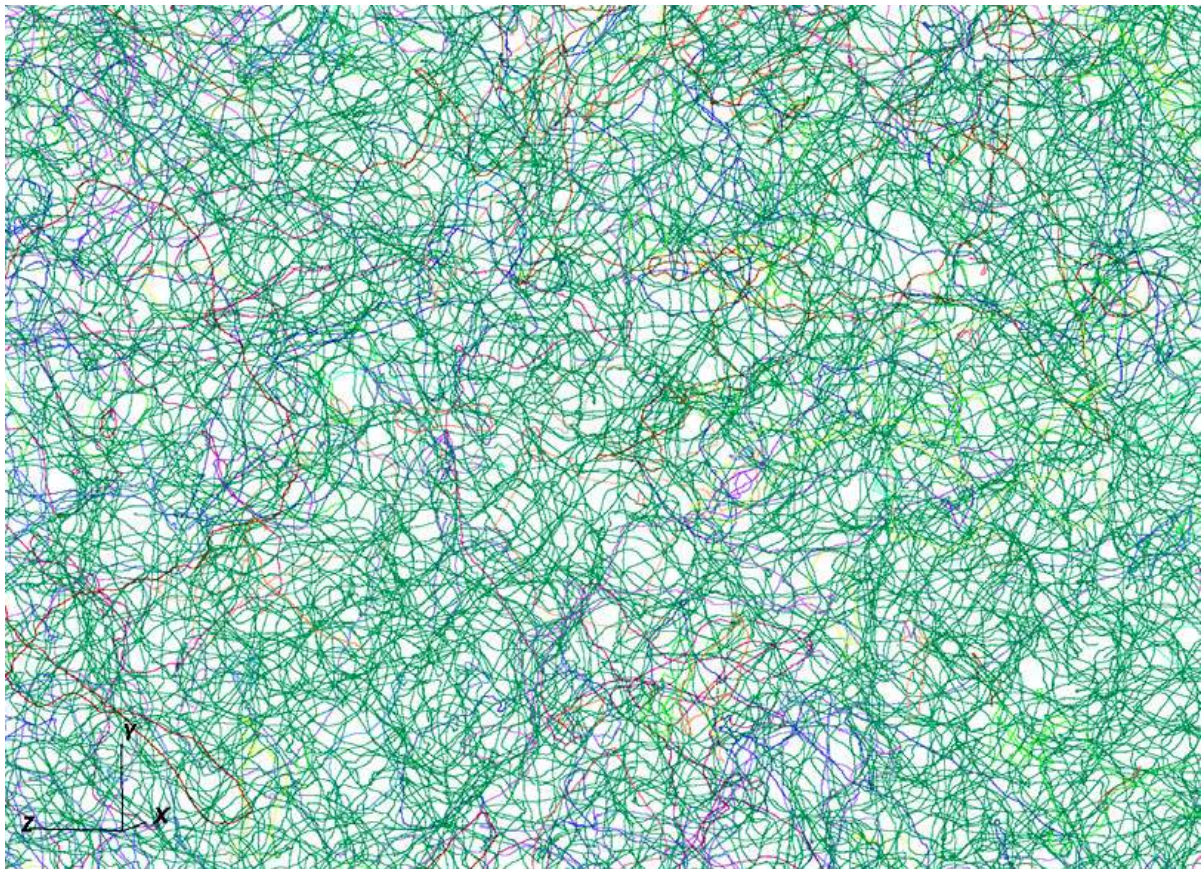
During the inflation phase, the young universe is supposed to have expanded extremely quickly at an exponentially increasing speed. In the models used, the phase of rapid expansion mostly ends with a phase transition that also leads to so-called symmetry breaking. Here, the basic forces of the strong and weak interaction and the electromagnetic force are supposed to have split into forces acting separately. According to the so-called Grand Unified Theory (GUT), these three basic forces had previously manifested themselves in a single force.

In their models, Martin Kunz and his team simulate cosmic strings during this phase transition. After all, it provides the ideal conditions for producing detectable cosmic strings as, at the time of the GUT symmetry breaking in the universe, an incredibly high energy level of 10^{16} gigaelectron volts prevailed – one billion times more energy than the large hadron collider at CERN can generate. According to the researchers, at such energy levels the defects are so strong that they should be detectable.

To detect the cosmic strings, the team thus simulates their location and distribution in different field conditions and measures their energy density. The results of the simulations are channelled into a programme that calculates the corresponding fluctuations in the cosmic background radiation using linearised equations. By comparing the results with the cosmic background radiation data, which the Planck satellite supplies during its mission, the researchers are hoping to be able to confirm these unusual defects. The cosmic background radiation may well only have originated 380,000 years after the Big Bang; however, it exhibits minimal fluctuations that, from what we know today, stem from the early universe. "If topological defects are present in the universe, they produce additional fluctuations that effectively contain a finger print of the defects and thus allow conclusions to be drawn as to their nature and origin," says Kunz.

Moment of truth draws closer

Martin Kunz's doctoral student David Daverio helped to improve the complex simulations significantly. In his Master's thesis, he completely rewrote the parallelisation of the codes used, which now means that the simulations can be carried out considerably more efficiently and a resolution that is sixty-four times higher achieved. This is an advantage for the researchers as time is of the essence. By 2014 at the latest, the results of the simulations need to be on hand so that they can be compared with the new Planck data. If the theories on the links between inflation, the formation of cosmic strings and the existence of a GUT are correct, this should be proved from the Planck data by then at the latest. Otherwise, once again it will be a case of excluding a model and trying to detect the supposed cosmic strings in another way – or bury them once and for all.



Zoom (64X) of the simulated cosmic strings network. The simulation have been running on the Cray XC30 Piz Daint on a torus with 4096^3 point and using 34816 cores (96% of Piz Daint). Each individual string is plot with different colors. We can see a very long string (dark green) which is wrap several times on the torus and which represent 10% of the network. (Image: David Daverio, Jean Favre)

Interview

Why are you researching cosmic strings?

That's a good question (laughs)! It all came about because I did a doctorate under Ruth Durrer in Geneva, who just happened to be researching defects at the time. It was a nice area for me since it's physics you know exists in condensed matter and you can transfer it to the universe and look for it. I find it very nice physics. It's interesting and I just enjoy figuring out the simulations. As it's something that exists, you get the feeling that you're not doing something completely pie in the sky. The concept of topological defects has some bearing on reality. Whether cosmic strings do remains to be seen.

What can cosmic strings explain in cosmology?

Originally, we wanted to explain why all the structures were formed in the cosmos but we and other groups discovered that this isn't possible. Meanwhile, for us cosmic strings are more a by-product of inflation, through which we want to close in on inflation. If we found cosmic strings, we'd have the possibility to learn a lot about physics at very high energy levels. The energy levels at which these develop are many billions of times higher than those that even Cern or we will ever be able to achieve on Earth. The only way to research such energy ranges is cosmology.

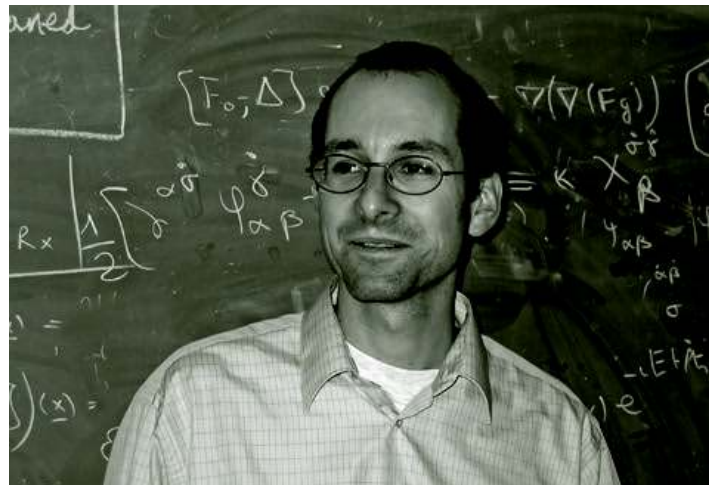
What uses could this research have?

Cosmology and astrophysics are something that always interests the general public and students. Even though basic research like ours is a far cry from what you need on a daily basis. In the past, however, quantum physics à la Heisenberg or Schrödinger was also basic research. You could scarcely imagine what you needed it for.

As cosmologists, we're really at the cusp of natural philosophy but, who knows, if we were able to explain inflation or find topological defects that revolutionised high-energy physics or explained dark energy, it could change physics to such an extent that we gain completely new insights. These, in turn, could well significantly change our lives much later.

So you assume that confirming cosmic strings could change our view of the world.

Yes, if we found cosmic strings, it would change and improve our understanding of the universe.



Martin Kunz is a professor in the Cosmology Group at the University of Geneva.

Can you give an example?

If the discovery is consistent with an inflation model on a GUT scale, it would be the first direct test of something connected with inflation. We would thus reinforce the model. On the other hand, it would also reinforce the concept of GUT itself and presumably help to find out what exactly the symmetry groups that are relevant are. This would give us a much better idea of what high-energy physics looks like at energy levels much higher than those Cern can generate. At the moment, the standard model is incomplete. Until something new is invented, no-one really knows what is between the Cern energy and that of quantum gravitation, which we can't even describe. We're talking about a desert here as no-one exactly knows whether anything happens in this range. If we found a direct relic from the other side of the desert, it would be able to tell us far more about what lies in between.

And what if we don't find this relic?

Then we'd shelve a couple more models.

But doesn't this put a question mark over the inflation hypothesis itself?

The way I see it, once we've got the data from the Planck, surely we'll be able to confirm or reject almost all the inflation models that are embedded in a GUT theory in two or three years. Our scenario of inflation is a specific implementation in particle physics. We can't do without inflation as such because we haven't got an alternative.

Solving the mystery of Neanderthal man on the supercomputer

An agent-based simulation is set to show how Neanderthal man and modern humans struggled for survival in an inhospitable era. The CSCS supercomputer “Monte Rosa” is to assess which of the current hypotheses can explain the extinction of the Neanderthals.

20,000 to 200,000 years before our time, at least two types of hominid were alive on Earth at the same time in the form of Neanderthal and modern man. Whereas modern humans in Africa and Neanderthals in Europe lived separately from one another, in the Middle East *Homo sapiens* and *Homo neanderthalensis* cohabited for around 100,000 years. Just why the Neanderthals suddenly died out more than 20,000 years ago remains unexplained to this day.

Gone in spite of common ground

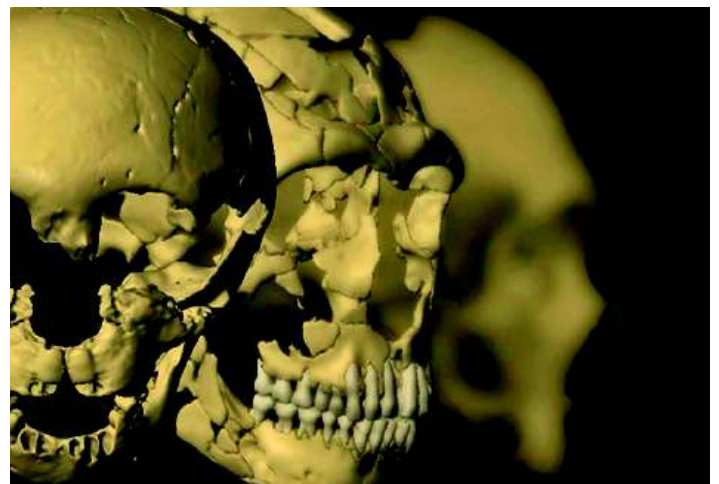
Modern humans came to Europe around 40,000 years ago, about 15,000 years before the Neanderthals disappeared for good. As DNA analyses of the Neanderthal genome show, the two species did have contact with one another: modern humans have up to four per cent Neanderthal genes. According to what we know today, the sociocultural behaviour of the two species had certain things in common: both species used tools and fire, buried their dead and engaged in rituals, such as painting their bodies with ochre. And both had the same sized brain. The extinction of the Neanderthals therefore poses scientists with many puzzles – puzzles that cannot be unravelled by experiments, but only based on facts that anthropologists collect through field work and fossil finds. Indeed, these provide indications of possible causes of the extinction of the Neanderthals, but no definitive explanation. However, it seems that the climate may have made a decisive contribution to their downfall.

Skeletal finds suggest that Neanderthals lived in Europe before the start of the last ice age – and for ten thousand years during it. However, during the peak of the ice age, which was characterised by strong climate fluctuations, they suddenly disappeared. The ice caps reduced the size of the available habitable area and the forests were replaced by grasslands. This changed the food that was available and led to different hunting conditions, which may have led to a situation where the Neanderthals, despite adapting to the harsh climate, were no longer able to meet their high energy needs. Different cultural and technical developments could also have helped modern humans to survive.

But the extinction of the Neanderthals may also have been a combination of these factors – or purely random.

Surviving because others died out

For Christoph Zollikofer, Professor of Anthropology at the University of Zurich, the key point of interest in relation to the phenomenon of extinction is the disappearance of populations. “The survivors do not survive because they are the fittest, but for the reasons that the others died out. That is an altered perspective that is rather unusual in the evolution of humans,” Zollikofer emphasises. In order to reassess Neanderthal extinction, he and his team are now pursuing new methods: with the aid of CSCS supercomputer “Monte Rosa”, they plan to simulate the extinction event in an agent-based model.



Computer simulations should help to explain why the Neanderthals died out. (Image: Research group Zollikofer)

Such models are increasingly gaining in importance in order, for example, to simulate human behaviour, such as in a mass panic. In this modelling technique (see box), each individual (human and animal) in the system to be modelled is represented as a discrete object. He, she or it is assigned specific characteristics such as height, gender, weight or energy consumption. Via an algorithm, the individual is also given the ability to seek food, interact with other individuals or move to other regions where better living conditions prevail. For this complex bottom-up approach, the scientists developed new codes and software, which are now to be adapted optimally to modern hardware.

The Swiss High Performance and High Productivity platform (HP2C) provides the ideal conditions for Zollikofer and his team. HP2C is an interdisciplinary cooperation between scientists, mathematicians, IT specialists and hardware manufacturers who are looking to adapt existing algorithms for modelling and answering complex scientific questions on future computer architectures in such a way that they can be used efficiently.

Support from the physical sciences and mathematics

Zollikofer praises the ideal conditions, but does not make a secret of how difficult it has been to put together a research team to take on this challenge. It was not from anthropology, but other disciplines that, after a long search, he and his colleague Jody Weissmann found support: from mathematician Wesley Petersen, astrophysicists George Lake and Simone Callegari, and biophysicist Natalie Tkachenko, who are now developing the codes for the model – a model that is supposed to unite short-term, local patterns of individual human behaviour and long-term, globally-acting patterns of changed environmental conditions. The researchers would like to use it to run through various behaviour scenarios between Neanderthals and humans, taking into account the fauna, climate conditions, topography and vegetation, in order to research the possible causes of the extinction of the Neanderthals in greater detail.

The agent-based models are to be combined with classic top-down diffusion models, which are used to research population dynamics.

“Among other things, we want to test the validity of agent-based models with them”, says Weissmann. Tkachenko is researching the coupling between the diffusion models and the agent-based models. “What we aim to model corresponds to the saying that the flapping of a butterfly’s wings in China can cause a tornado in the USA,” says Zollikofer. He points out that, so far, no-one has tested whether something like this is possible: whether – analogously to the flapping of a butterfly’s wings – the local behaviour of a single individual could have effects on the entire human population.

Reducing a simulation period of years to a few weeks

With their project, the team would like to find out to what degree of detail the simulation of such complex relationships is possible. In order to obtain meaningful results, each simulation must be carried out with tens of thousands of single individuals several hundreds of times and with differing starting conditions. Developing the prototype for the model for this would take years.

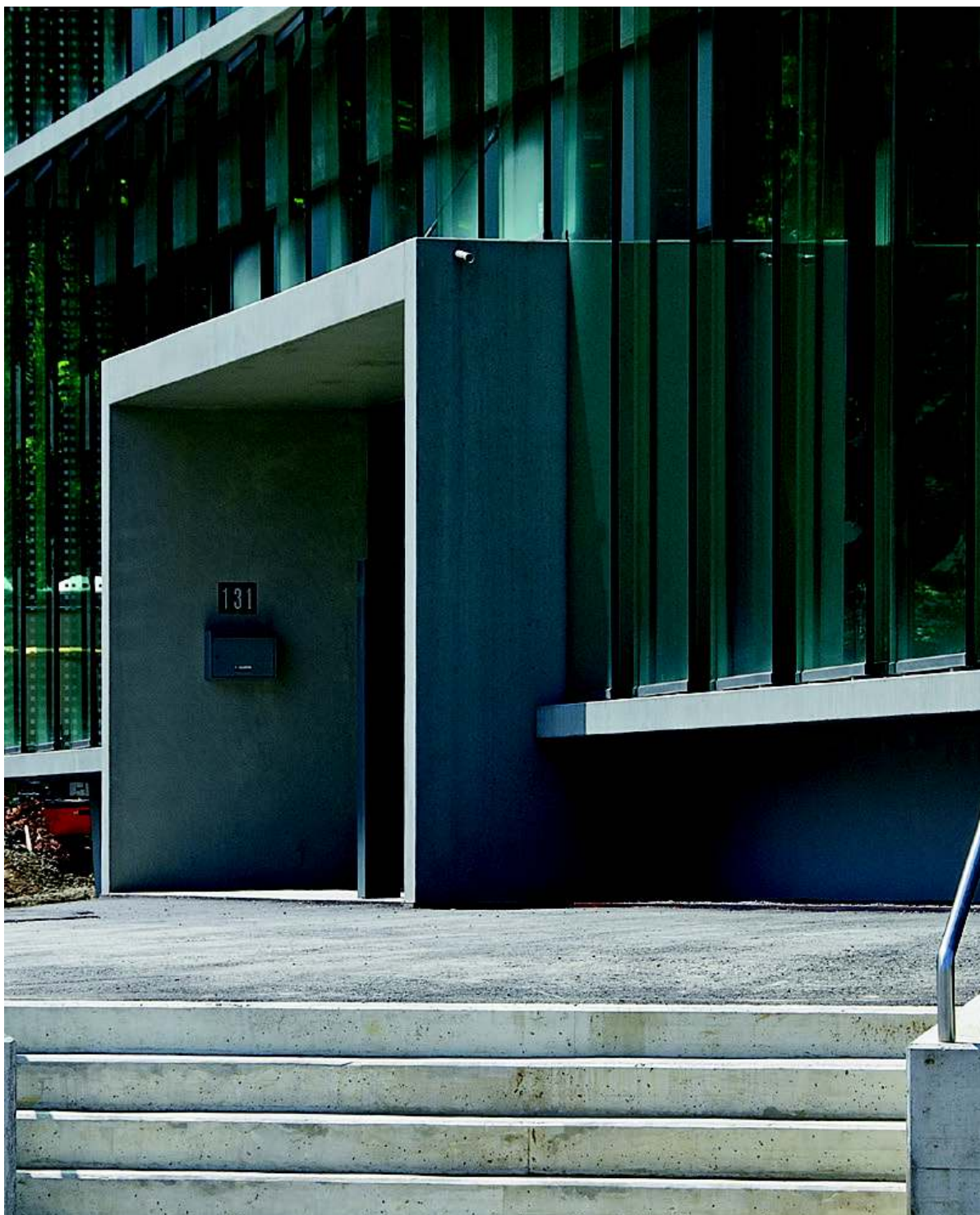
Through the interdisciplinary cooperation within the framework of HP2C, however, Zollikofer and his team would like to carry out the simulations in a few months or weeks. The professor is convinced that such massively parallel, multi-agent-based simulations will become increasingly important in the question as to the effect of migration in the modern world or an evacuation in the event of a reactor accident, for example.

Agent-based modelling

The agent-based modelling method is used in different areas where complex systems are to be modelled, such as to predict how the shares market will develop, an epidemic will spread or, looking back, investigate the decline of civilisations. The method is based on the simulation of the interaction of autonomous agents with one another and their environment. The behaviour of the agents is described by simple (if-then) rules and complicated (adaptive artificial intelligence) ones. Assigned to each are different characteristics and modes of behaviour, through which they all differ from one another. The modelling of each individual and their interaction shows how patterns, structures and behaviours can develop that were not pre-programmed. This self-organisation only develops through interaction.

In order to determine the spatial movement of a Neanderthal individual, the researchers place it, as an agent in their model, in the centre of a cell that is shaped like a honeycomb. To each cell, they assign particular values for the topography, climate, available food and potential enemies. The cells make up a honeycomb grid. On it, the agent determines in which direction it will most probably move.

The test runs on twenty CPUs, in which the interaction of a million “simple” agents is simulated in 100,000 simulation steps that take two days. Here, one simulation step corresponds to a period of one day to around a week. The aim, however, is to simulate 10 million more complex agents with 1 million simulation steps and 1,000 repetitions. Under the aforementioned conditions, that would currently take 600 years.



The entrance of the new CSCS building in Lugano.

Papers with Highest Journal Impact Factor¹⁾

Nature

Impact Factor: 36.28

T. Rutishauser, R. Stöckli, J. Harte, L. Kueppers, Climate change: Flowering in the greenhouse, *Nature*, DOI: 10.1038/485448a.

Nature Materials

Impact Factor: 32.84

D. Meier, J. Seidel, A. Cano, K. Delaney, Y. Kumagai, et al., Anisotropic conductance at improper ferroelectric domain walls, *Nature Materials*, DOI: 10.1038/nmat3249.

Science

Impact Factor: 31.20

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INAUGURATION OF THE NEW BUILDING IN LUGANO

Big day for CSCS in 2012

After a two-year construction period, the new building for the Swiss National Supercomputing Centre (CSCS) in Lugano was officially inaugurated by Alain Berset, a member of the Swiss Federal Council, on 31 August 2012.



Federal Councillor Alain Berset cut the symbolic ribbon together with Fritz Schiesser, President of the ETH Board (left), and Ralph Eichler, President of ETH Zurich and host of the event (right).

“The investment in this infrastructure is a long-term commitment to world-class research and part of an education and research policy that is designed to make a lasting contribution to the wellbeing of the country.” With these words, Federal Councillor Alain Berset opened the new CSCS building on 31 August 2012.

Insight into the world of HPC and its benefits

Around eighty invited guests from the worlds of politics, business and science took part in the official ceremony and seized the opportunity to visit what is currently one of the world’s most energy-efficient computing centres, where the computers are cooled using water from Lake Lugano. While Federal Councillor Alain Berset, President of the ETH Board Fritz Schiesser and President of ETH Zurich Ralph Eichler explained the significance of the supercomputing centre for Switzerland and research to the guests in their speeches, CSCS Director Thomas Schulthess spoke about the development of supercomputing in the past twenty-four years and provided an insight into the strategy that the centre wishes to pursue in years to come.

He emphasised the fact that the computer power, which has ballooned by a factor of one thousand every ten years during this period, went hand in hand with a constant increase in energy consumption – one of the reasons why the new building became necessary. Schulthess wants to use CSCS to focus on technologies in future that not only provide optimum computational power for the users, but also help curb electricity consumption. Domenico Giardini, a professor of seismology at ETH Zurich, delivered a particularly exciting talk at the ceremony, in which he described to the guests how supercomputers have supported research. When he showed a simulation of how earthquake waves spread out along the San Andreas Fault in California and the colour intensities pulsating in the film demonstrated the force of the quake in different regions, even a lay person could quickly recognize the areas particularly at risk.

Recognition of positive development

CSCS was given a special mention in the lecture by Horst Simon, Associate Laboratory Director at Lawrence Berkeley National Laboratory, in which he spoke about the development of supercomputing in Switzerland. He highlighted the importance of projects such as High Performance and High Productivity Computing (HP2C) alongside the supercomputing infrastructure. The project, which, like the new building, was made possible by the HPCN Strategy, creates a network for researchers from different universities and research institutes where they can work together on preparing the software they use for future computer technologies and making it more efficient.



Federal Councillor Berset (left) inspects the computer building under the guidance of CSCS Director Thomas Schulthess (front right); in the background, President of the ETH Board Fritz Schiesser.

Overwhelming visitor numbers

The huge interest of the public in the new building and the work of CSCS was a source of great surprise. CSCS is responding to this interest with more public events.

On the day after the official opening, CSCS opened its doors to the general public. Far in excess of 2,000 people from all over Switzerland and Northern Italy took the opportunity to visit the centre's new premises. The scientists and employees at CSCS gave the visitors an insight into what high-performance and scientific computing entails.

Those who managed to find a spot in one of the two large conference rooms at CSCS despite the flood of visitors got a behind-the-scenes look at the basic remit and work of CSCS or were able to find out more about the Large Hadron Collider and the new particle recently discovered at CERN, which in all probability is the elusive Higgs Boson. But other topics on the programme also included astronomy, climate and seismology using supercomputers. The scientists and employees at CSCS were available for question-and-answer sessions with the audience after the lectures. At the same time, there were guided tours of the building and CSCS staff provided visitors with a better insight into areas such as the world of simulations, materials research and cosmology, and the history of supercomputing.

The flow of visitors continued unabated until the evening. As a result, since then CSCS has been offering guided tours on request and organising scientific colloquiums where researchers report to the public on their research with supercomputers. This service is proving very popular and public interest continues to be great – both on the guided tours and in the colloquiums.



The audience of astrophysicist Marcella Carollo.



A visitor in discussion with Thomas Stocker, a climatologist at the University of Bern.



Food and drinks tent: visitors were catered for with risotto and drinks in a tent in CSCS car park.

Taking the tour of the building.

Scientific community-driven development of supercomputing systems

The Swiss High-Performance Computing and Networking strategy is investing in three areas: supercomputing systems, the necessary data centre infrastructure and a competence network for application development. While the first two are straightforward to conceptualise, it is far from obvious how the application development for high-end simulations on modern supercomputers has to be organised. To this end, the High-Performance and High-Productivity Computing platform (HP2C, see www.hp2c.ch) provided a first systematic step towards a competence network. The HP2C invested in twelve application development projects from 2009 to 2012 that were selected in an open call at Swiss universities and federal institutes of technology. These projects formed the nucleus for domain science community networks that were formed following a second open call in late 2012. The five networks (see sidebar) include over forty research groups across Switzerland and cover physics, atmospheric science (climate and meteorology), geophysics, (quantum) materials science and chemistry, and life science. They will form the basis upon which the Platform for Advanced Scientific Computing (PASC) will be built with support from the Swiss University Conference (SUK) in the years 2013-2016.

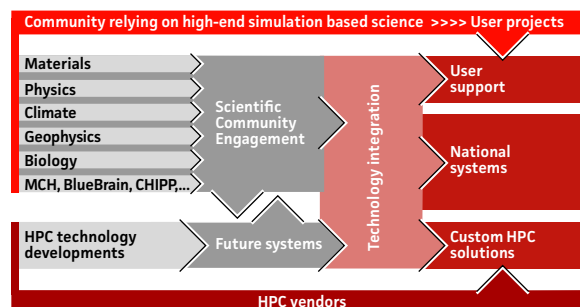


Platform for Advanced Scientific Computing

The main thrusts of the SUK-funded PASC are the development of the domain science networks and co-design of future high-end simulation systems with CSCS and the supercomputing industry. The domain science networks are responsible for developing scientific roadmaps for grand challenge problems that are well beyond the horizon for individual research groups but can be tackled with appropriate interdisciplinary efforts in the next five to ten years. Furthermore, the communities are expected to liaise with computer scientists and applied mathematicians, as well as CSCS and computer manufacturers, in order to identify key technologies that need to be developed to implement the scientific roadmaps on new and emerging computing architectures. PASC will support the development of these technologies through co-design projects, a call for which will be published at the beginning of 2013 (see www.pasc-ch.org).

Since the autumn of 2011, CSCS has been adapting its organisational structure and processes in order to enable the scientific-community-driven development of future supercomputing systems. The goal is to foster the design of the supercomputing systems of the user lab from use cases defined by the PASC communities and using the capabilities developed by co-design projects. The process is depicted in the figure above (or below). Members of the scientific community engagement section collaborate with the domain science communities, as well as key customers of CSCS such as MeteoSwiss, the Blue Brain Project at the EPFL or the Swiss Institute for Particle Physics (CHIPP), in order to articulate the roadmaps and their implications for computing system needs. At the same time, the Future Systems group engages with computer systems research teams in academia and the computer industry in order to identify possible hardware and software solutions based on new and emerging computer architectures. The two groups, community engagement and future systems, collaborate on the development of prototype solutions. Prototypes will include novel hard- and software – domain specific libraries and tools as well as more generic numerical libraries and programming environments. Successful prototypes will be combined into projects led by the Technology Integration section that will result in simulation systems and new supercomputers for the centre. Depending on their purpose, these computing systems will be operated by one of the two respective systems groups at CSCS, the National Systems group and the Custom HPC Solutions group. The User Support group works with users of all CSCS systems and runs the allocation process on the systems of the national user lab. User Support, Scientific Community Engagement and Future Systems staff collaborate closely in order to provide the scientific community and society with the most up-to-date knowhow on new and emerging computing architectures.

CSCS with co-design



Ben Moore joined the University of Zurich in 2002 to establish a new research activity in astrophysics and cosmology. His research focuses on the origin of structure in the Universe, from planets and stars to galaxies, on which he has penned over 200 scientific articles. The Zurich group has designed and maintains several state-of-the-art computational astrophysics codes used by researchers worldwide.



Isabelle Bey is the Executive Director of the Center for Climate Systems Modeling (C2SM). C2SM is a research center jointly established and funded by ETH Zurich, MeteoSwiss, and Empa, with the main objective to improve the understanding of the Earth's climate and weather systems and our capability to predict it. The Center fosters the collaboration between the partner institutions and maintains and disseminates key climate models and datasets.



Nicola Marzari holds the Chair of Theory and Simulation of Materials at the EFPL, having joined in 2011 after many years at MIT (most recently as Toyota Chair of Materials Engineering) and the University of Oxford, where he held the first statutory (i.e. University) Chair of Materials Modelling. His research is dedicated to the development and application of quantum simulations and outstanding problems in materials science.



Petros Koumoutsakos was elected as an assistant professor in 1997 and has been a full professor of computational science at ETH Zurich since 2000. He was founding director of ETH Zurich's Computational Laboratory (2001-2008) and served as Head of the Institute of Computational Science (2002-2006). He is an elected fellow of the American Physical Society and the American Society of Mechanical Engineers.



Tarje Nissen-Meyer has been a research scientist at ETH Zurich since 2010 and will join Oxford University as a university lecturer in 2013. An expert in computational seismology, he was instrumental in the HP2C project Petaquake. Previously, he held research positions at Princeton University and California Institute of Technology. He received a PhD from Princeton University after studying geophysics at LMU Munich and McGill University.



Finances

Expenditures

	CHF
Investments	17 320 218.42
Material / Goods / Services	215 621.88
Personnel	6 388 608.44
Payroll	5 026 061.70
Employer's contributions	852 526.10
Further education, travel, recruitment	510 020.64
Other Material Expenses	5 885 978.90
Maintenance Building	576 949.35
Energy & Media	1 834 774.76
Administrative expenses	41 590.35
Hardware, Software, Services	2 649 685.91
Remunerations, Marketing, Workshops	
Services, Technical Move	775 599.17
Other	7 379.36
Extraordinary Income / Expenditures	150 712.00
Membership fees / Overhead	150 712.00
Total Expenses	29 961 139.64
Balance	

Income

	CHF
Basic Budget	34 322 643.10
Contribution ETH Zurich	15 740 000.00
BM BFI-Botschaft HPCN	18 500 000.00
Salary Increase / Price Inflation / PK	78 822.00
Account Transfers	3 821.10
Other Income	78 633.72
Services / Courses	22 756.57
Reimbursements	13 233.95
Sponsorship / Others	42 643.20
Total Income	34 401 276.82
Balance	4 440 137.18
Third party contributions	
CRUS	904 912.65
ETH Board	118 000.00
European Commission	191 758.80
MeteoSwiss	1 178 000.00
Switch	32 500.00
SystemsX	80 000.00
USI	645 372.00
Other	16 000.00

Development of Overall Expenses

	2009	2010	2011	2012
Investments	11 540 846	8 417 349	15 777 324	17 320 218
Personnel	6 284 972	7 534 853	7 530 745	6 388 608
Other Material Expenses	5 399 155	6 706 740	4 818 411	6 825 156

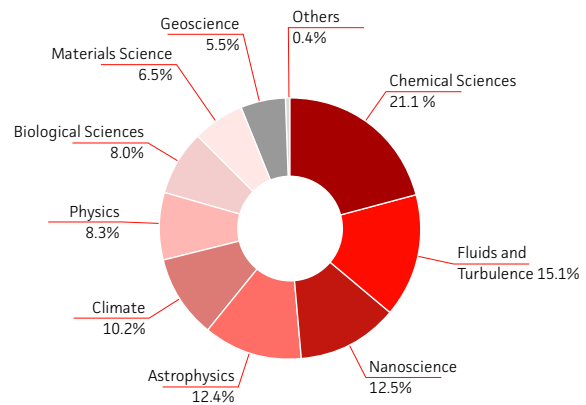
Mio CHF



Usage statistics

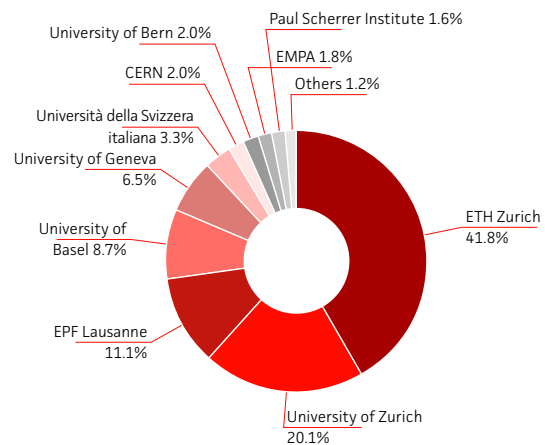
Usage by Research Field

Research Field	CPU h	%
Astrophysics	33 566 053	21.0
Biological Sciences	21 787 884	15.1
Chemical Sciences	57 389 129	12.5
Climate	27 610 355	12.4
Fluids and Turbulence	40 979 832	10.2
Geoscience	15 030 977	8.3
Materials Science	17 772 339	8.0
Nanoscience	33 933 906	6.5
Physics	22 432 428	5.5
Others	969 858	0.4
Total Usage	271 472 761	100.0

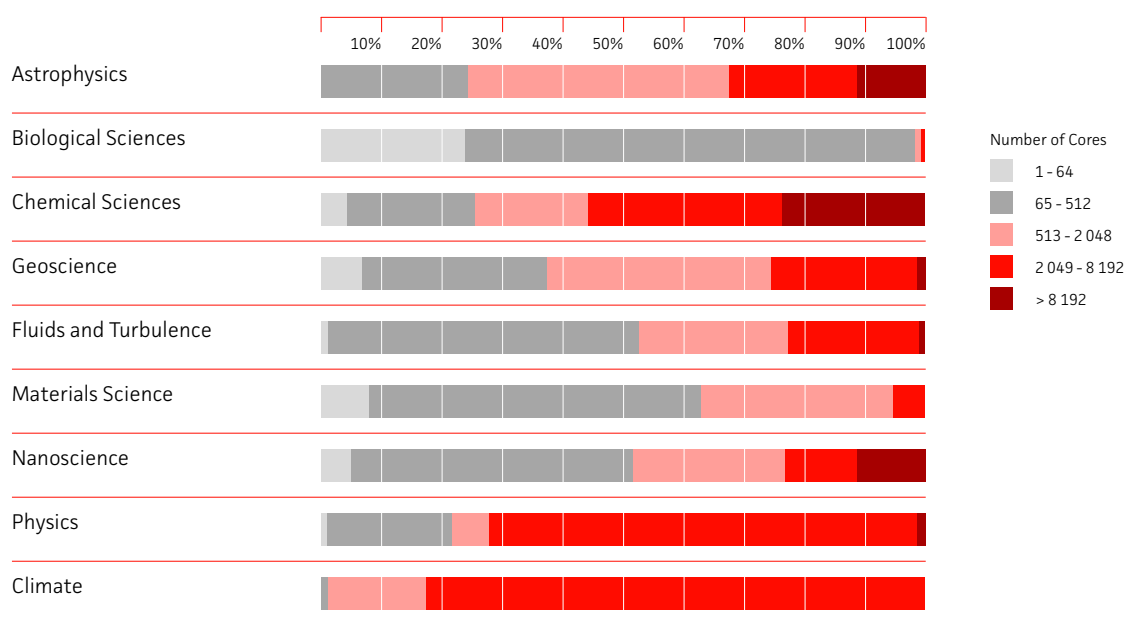


Usage by Institution

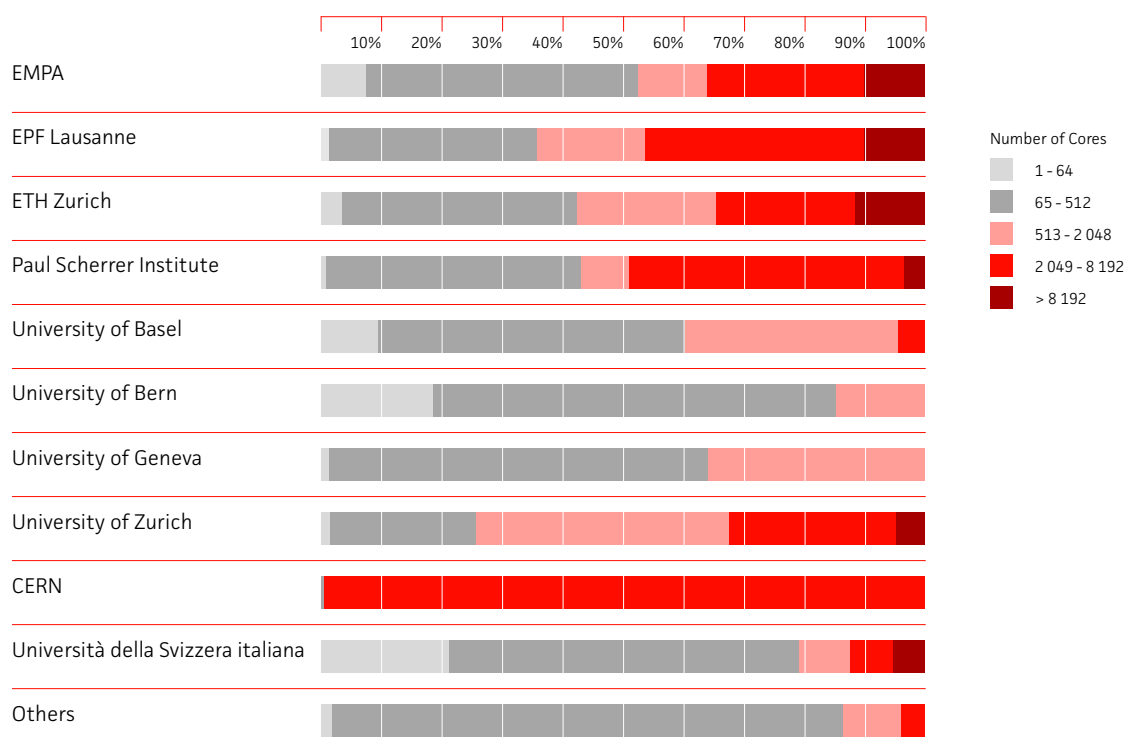
Institution	CPU h	%
ETH Zurich	113 487 216	41.8
University of Zurich	54 457 966	20.1
EPF Lausanne	30 161 173	11.1
University of Basel	23 584 744	8.7
University of Geneva	17 588 918	6.5
Università della Svizzera italiana	9 022 267	3.3
CERN	5 334 162	2.0
University of Bern	5 364 190	2.0
EMPA	4 867 562	1.8
Paul Scherrer Institute	4 293 449	1.6
Others	3 310 814	1.2
Total Usage	271 472 461	100.0



Job Size by Research Field (in Cores)



Job Size by Research Institution (in Cores)



Compute Infrastructure

HPC Systems

Name	Supplier & Model	Installation / Upgrade	Usage / User	(h) Capacity Allocation Unit	Produced Allocation Unit	Availability (%)
Piz Daint	Cray XC30	2012 ¹⁾	National User Lab	12 994 560.00	9 495 023.00	-
Monte Rosa	Cray XE6	2009 / 2011	National User Lab	356 454 912.00	347 061 563.06	93.89
Tödi	Cray XK7	2009 / 2012	R&D	81 336 529.92	36 877 645.92	94.74
Monte Lema	Cray XE6	2012 ²⁾	MeteoSwiss	15 591 398.40	7 910 003.00	99.73
Phoenix	Sun Cluster	2007 / 2012	CHIPP (LHC Grid)	13 691 270.00	12 075 105.00	97.90
Pilatus	Intel Sandy Bridge Cluster	2012	National User Lab	7 862 976.00	1 143 067.50	99.59
Albis	Cray XE6	2012 ²⁾	MeteoSwiss	7 795 699.20	2 377 178.00	99.68

Name	CPU Type	No. of Cores	Interconnect Type	(TFlops) Peak Performance	(GB/s) Bisection Bandwidth
Piz Daint	Intel Xeon 2 E5-2670 2.6 GHz	36 096	Cray Aries	750.0	4050
Monte Rosa	AMD Opteron 6272 Interlagos 2.1 GHz	47 872	Cray Gemini	402.0	1920
Tödi	AMD Opteron 6272 Interlagos 2.1 GHz & Nvidia Tesla K20X GPU	4352 + 272 GPUs	Cray Gemini	393.0	760
Monte Lema	AMD Opteron 6172 2.1 GHz	4032	Cray Gemini	33.9	640
Phoenix	AMD Opteron 6272 2.1 GHz & Intel Xeon CPU E5-2670 2.6 GHz	2208	Infiniband QDR PCI Gen 2	21.5	144
Pilatus	Intel Xeon E5-2670 2.6 GHz	704	Infiniband FDR PCI Gen 3	14.6	300
Albis	AMD Opteron 6172 2.1 GHz	1728	Cray Gemini	14.5	360

¹⁾ Only December 2012

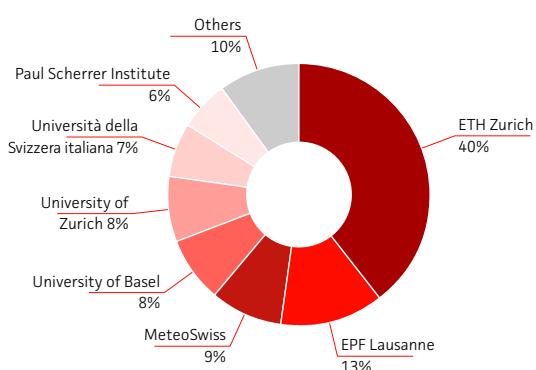
²⁾ Started production on July 1st, 2012

User Satisfaction

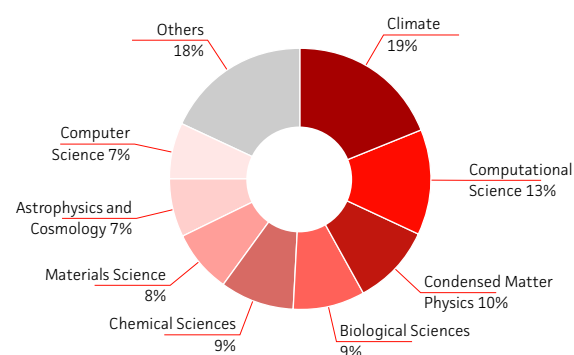
A user satisfaction survey was submitted to 842 users in January 2013. The response rate was of 29% (244 answers).

User Profile

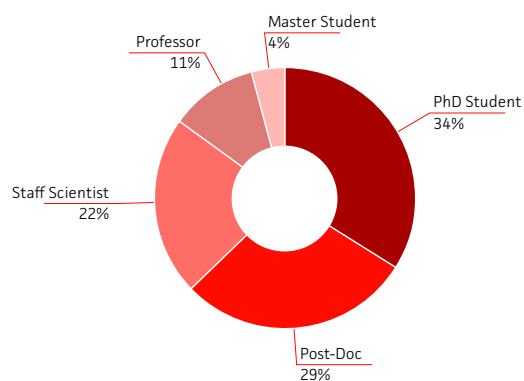
Your institution



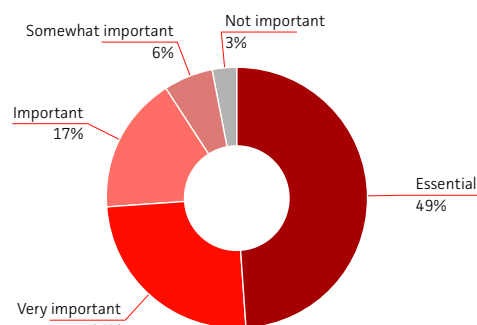
Your scientific field



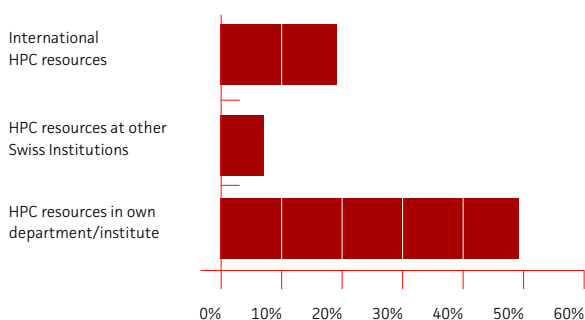
Your position

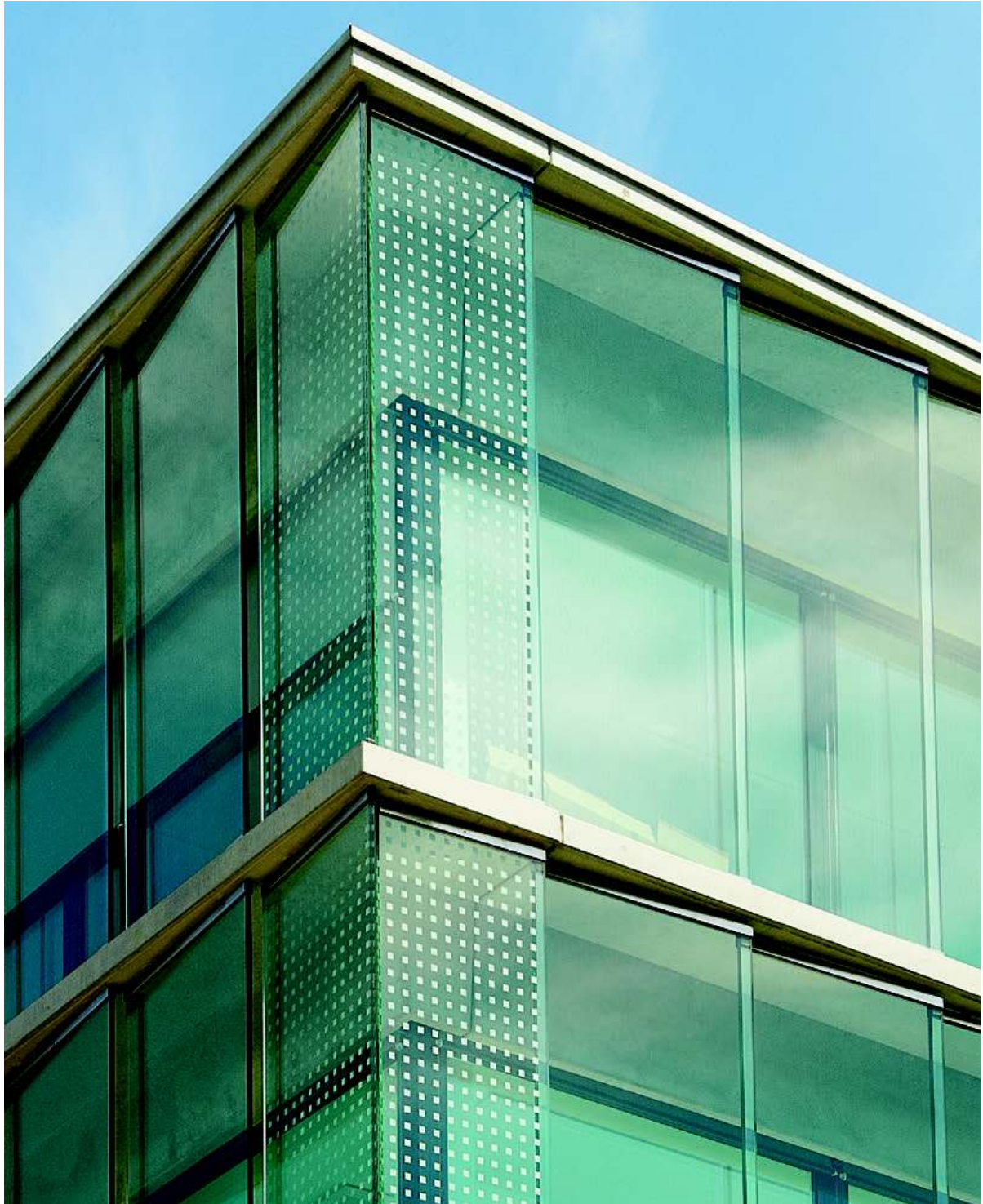


For my research, CSCS resources are



Which HPC resources are you using besides CSCS?





User Support

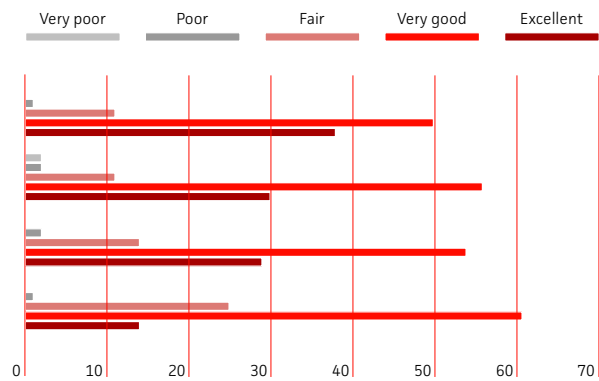
How do you rate the quality of...

Helpdesk support

System support

Application support

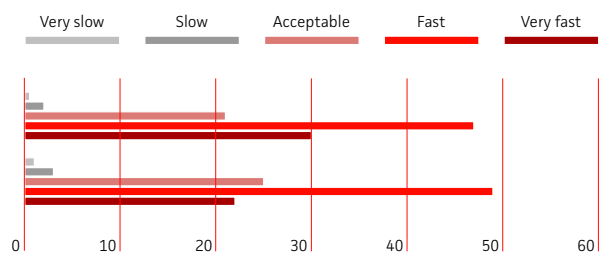
The offer of training courses and user events



How fast does support handle your request?

The reaction time of the helpdesk is

The time to solution for the support requests is



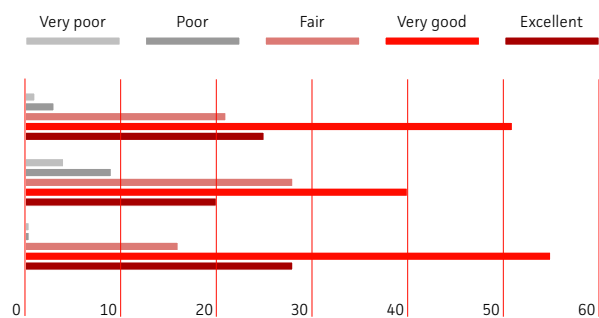
System Availability, Stability and Usability

How you perceive...

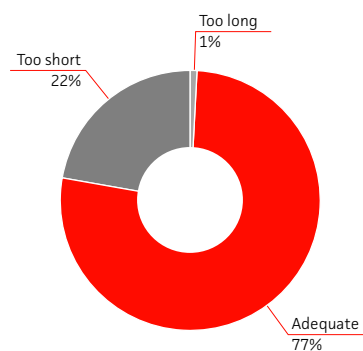
The availability of CSCS systems?

The stability of CSCS systems?

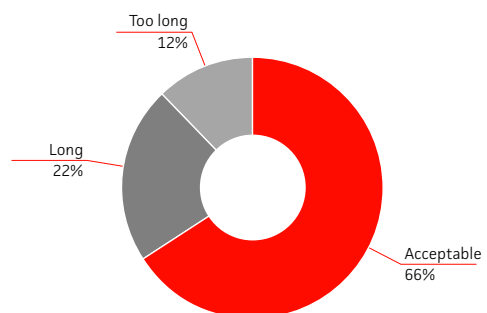
The ease of use of CSCS systems?



The run time limits for batch jobs are:

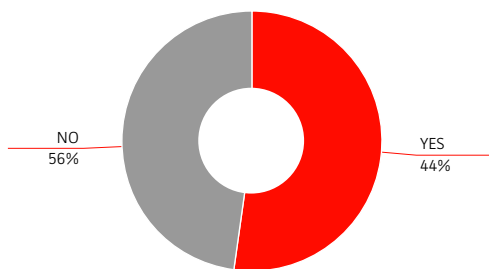


The job waiting time in the queue is:

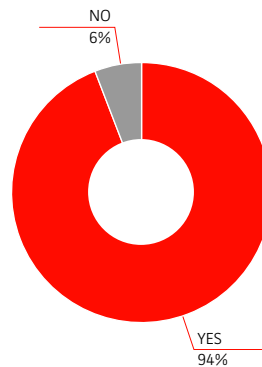


Project Proposal Process

Do you submit project proposals to CSCS (as PI or supporting the PI)?



Is the reviewing process transparent?



How do you perceive the submission process?

The submission portal is

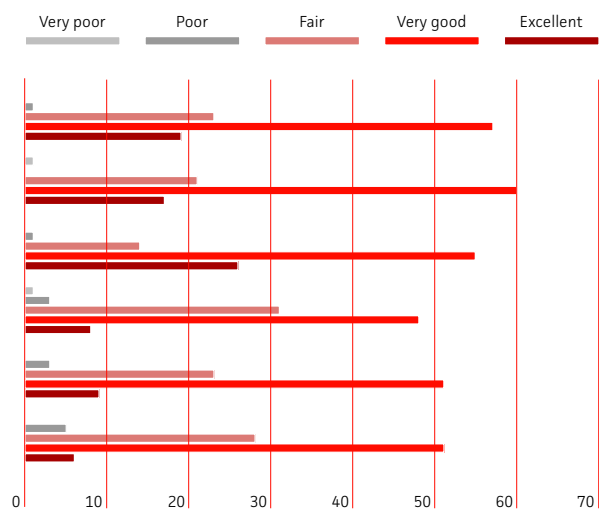
The quality of the submission form is

The support provided during the call is

The feedback from scientific reviewers is

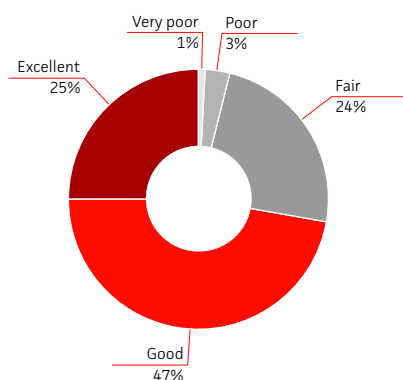
The feedback from technical reviewers is (when given)

The information provided by the panel committee is

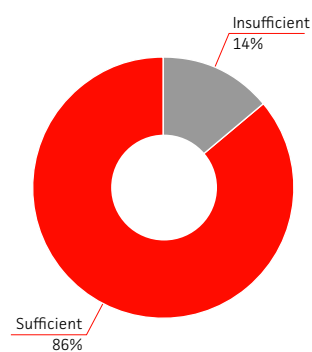


Adequacy of Allocated Resources

The resources assigned to my project are:

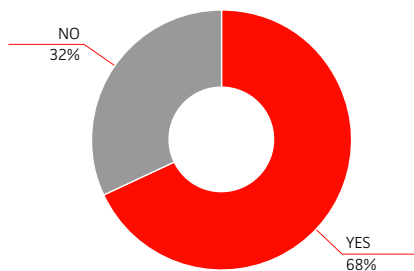


My storage allocation on /project is:

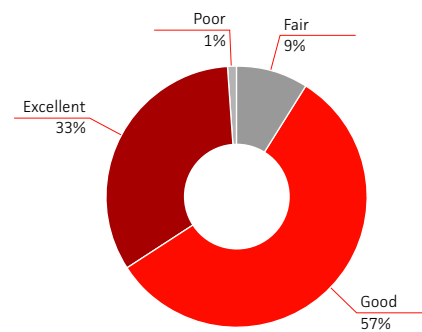


Application Development

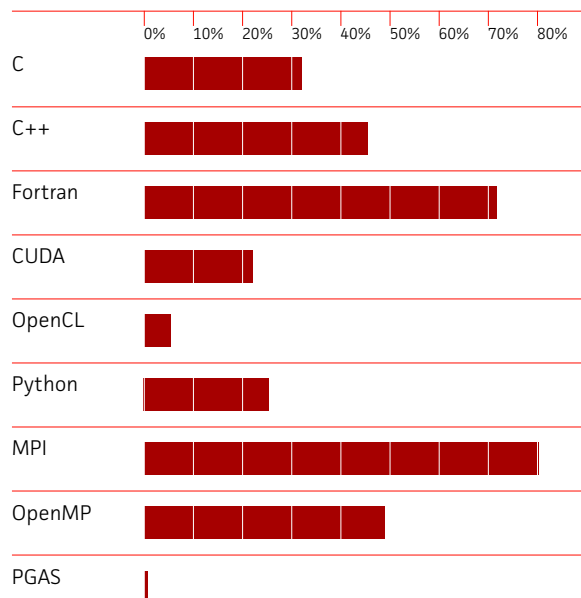
Do you develop and maintain application codes?



How do you rate the offered range of programming tools (compilers, libraries, editors, etc.)?

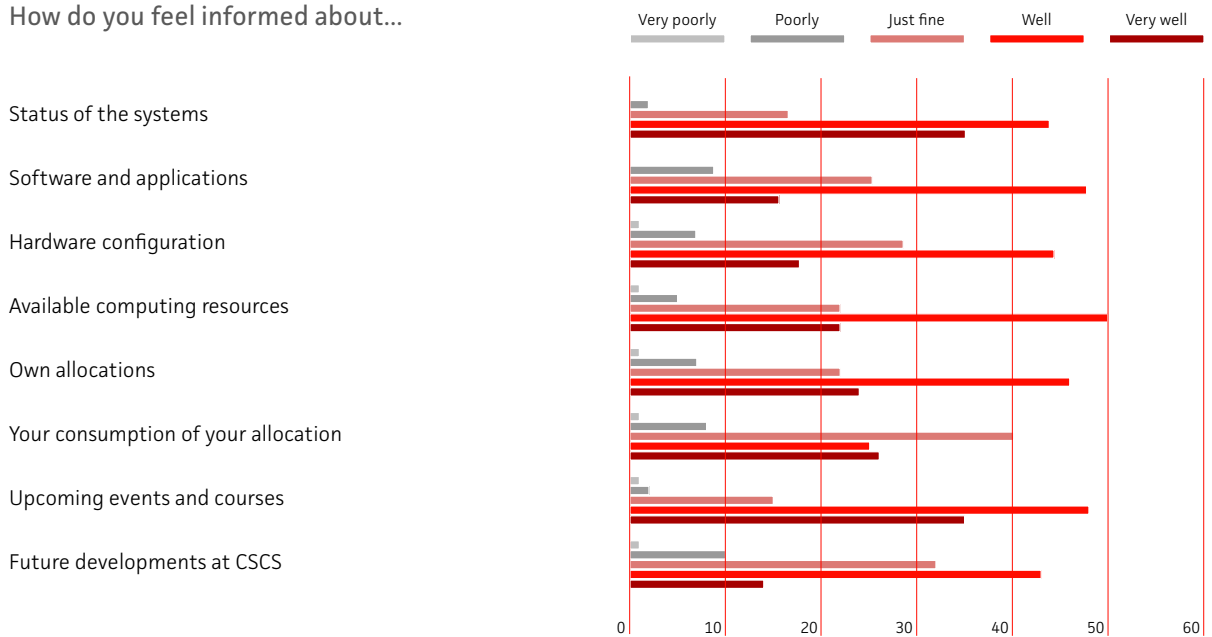


Which programming languages and parallelization paradigms are you using primarily?

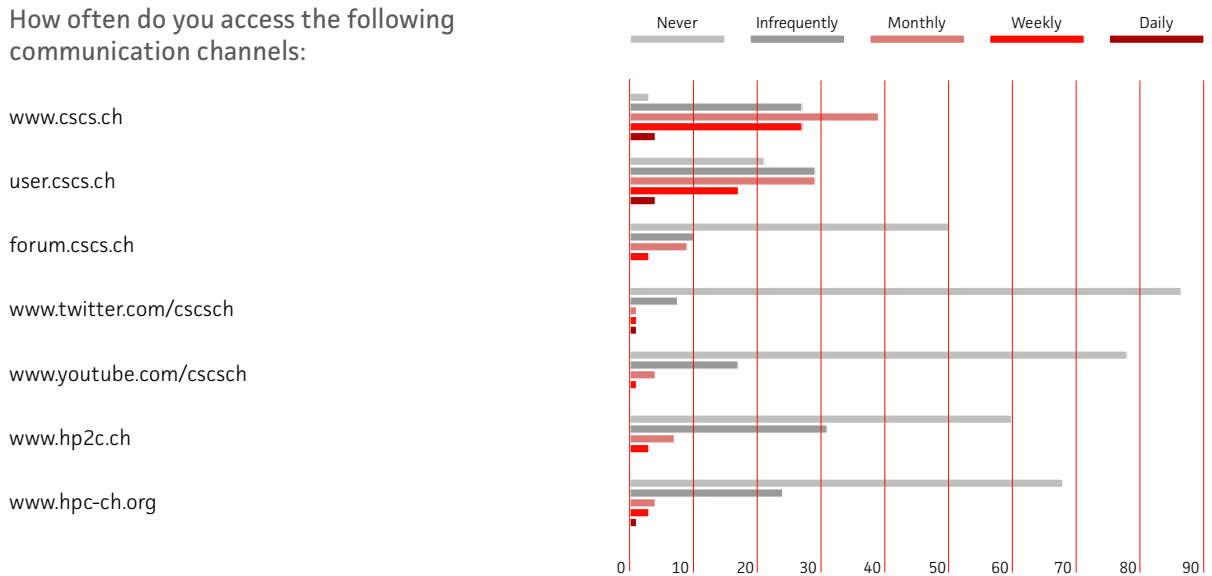


Information & Communication

How do you feel informed about...

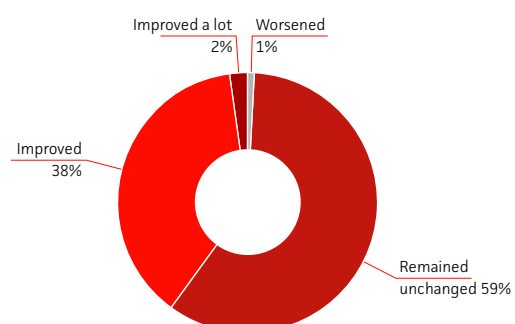


How often do you access the following communication channels:

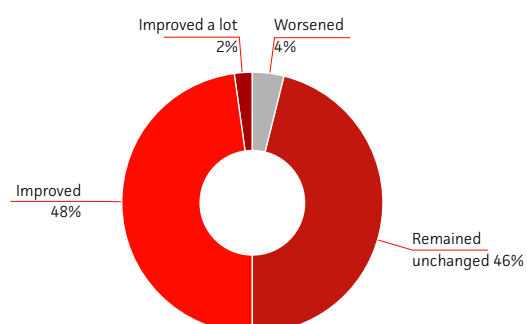


Perception of CSCS

How has the communication between CSCS and the user community developed during last year?



My general view in the last year is that CSCS (systems, services, support) has:



A detail of the new CSCS building in Lugano.

Impressum

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